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WELCOME...

In this riveting edition of Scientia, we showcase the work of many dedicated researchers across the globe who are solving the world's greatest challenges through engineering and technology research.

To open the edition, we feature an exclusive interview with representatives of the Natural Sciences and Engineering Research Council of Canada (NSERC) about the latest Gender Summit, whose aim is to make equality in research and innovation the norm. Here, we speak with the chairholders of the Chairs for Women in Science and Engineering Program, along with NSERC's president, who discuss some of the key outcomes of the Summit, the latest success stories and the challenges ahead for achieving full equity within the STEM community.

Our first section showcases the latest research into clean energy technologies. Here, we feature a selection of promising projects, from developing thermoelectric generators, which convert wasted heat into electricity, to ensuring the safe implementation of marine renewable energy technologies. Such research efforts promise to reduce and even eliminate our reliance on fossil fuels, in an effort to curb the most devastating impacts of climate change.

Next, we feature a collection of research initiatives that aim to develop innovative sensor technologies. Such novel sensors can help us address many significant societal challenges, from making healthcare more accessible to preventing environmental damage.

Our third and fourth sections celebrate two crucial fields within the world of engineering – fluid mechanics and materials engineering. Here, we meet an ensemble of dedicated engineers, who are driving progress in these fields towards diverse real-word applications, from semiconductors to aviation to building construction.

Last but not least, we celebrate the researchers who are spearheading the latest innovations in computing technology and data science. An overarching theme that pervades our final section is utilising the latest computing technologies in the quest to drive scientific discovery.



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OUTCOMES OF GENDER SUMMIT 11, CO-HOSTED BY NSERC







From November 6 to 8, 2017, more than 675 advocates of gender equity from across many different fields in science, technology, engineering and mathematics (STEM) took part in Gender Summit 11, in Montreal, Quebec.

Co-hosted by the Natural Sciences and Engineering Research Council of Canada (NSERC) and Fonds de recherche du Québec, the Gender Summit's aims were to highlight the importance of diversity and to share best practices for how to eliminate barriers faced by under-represented groups, such as women, in the STEM community. Under the overarching theme of 'Embracing pluralism and thriving through diversity – shaping science and innovation', the Summit's participants had the opportunity to engage in many important discussions, from how to reduce conscious and unconscious bias on hiring committees, to how to boost the number of women in leadership roles.

In this exclusive interview, we had the pleasure of speaking with Dr Catherine Mavriplis, Dr Tamara Franz-Odendaal and Dr Annemieke Farenhorst, chairholders of the Chairs for Women in Science and Engineering Program, along with NSERC's president, Dr B. Mario Pinto. Here, they share some of the key outcomes of the Summit, highlight the latest success stories and discuss the challenges ahead for achieving full equity in the STEM community. 'The research has shown that diversity of opinion leads to much better decision-making, unusual decision-making and non-linear thinking

 if I can put it that way – where you have different viewpoints and perspectives brought to bear on solving a particular problem.'



To start, could you briefly explain the overall aim and vision behind Gender Summit 11?

Dr B. Mario Pinto: Yes, I can. But, first, let me preface my comments by saying that the Gender Summit has been going on for a while. We joined the program at Gender Summit 3, and we've been participating in the other Summits. But by attending those Summits, I realised that we have to broaden the discussion beyond the differences in biological sex – between male and female. We really have to look at the other conflating factors of culture, ethnicity and other sources of diversity.

And so, when we put in our bid to run the North American conference, we decided that we would expand the theme of the Gender Summit to include pluralism and inclusion in all its aspects. With that in mind, the overall vision was to embrace diversity and to have a discussion of the other factors that would affect the gender balance in hiring, business, academia and so on.

It really is a very complicated, multivariable equation, if one considers different cultures at play, different races, different ethnicities, etc. That's why we put together this fairly broadlybased programme. I would be remiss if I didn't mention the indigenous aspect. So, we arranged specifically to hear from indigenous peoples and to consider their points of view as we debate the broader issues of gender equity and inclusion. Women are still under-represented in science and engineering. Explain how equality and diversity add to the scientific and engineering community and increase the relevance and quality of the research.

Dr B. Mario Pinto: The research has shown that diversity of opinion leads to much better decision-making, unusual decision-making and non-linear thinking – if I can put it that way – where you have different viewpoints and perspectives brought to bear on solving a particular problem. This is true in an academic setting, but it's also true in a business setting where, a report by McKinsey and Company has definitely shown that incorporation of diverse opinions and peoples in companies leads directly to economic gain, and there's now been a correlation shown between gross domestic product (GDP) and diversity.

On the academic side, there are many cutting-edge problems that need to be attacked, and here, too, one needs a diversity of perspectives. If one thinks the same way and one has no fresh input, what you get is a propagation of the same way of thinking. So, really, what you want is disruptive thinking. And that disruptive thinking usually comes from very diverse perspectives. We know that different people think very differently because of their backgrounds.

In terms of science and engineering, we have many global challenges. To solve them in a reasonable timeframe, I think



we have to join forces and embrace diversity of opinion and thought so that we can proceed toward the end goal. Definitely, we can show that the impact of the research is much higher when you have different points of view brought to bear on a particular problem. So, it comes about by looking at evidence, looking at research, and coming to the logical conclusion.

Dr Catherine Mavriplis: I would say that things have changed a lot over the last few decades. There are certainly some fields of engineering, in particular, that are doing really well because of the inclusion of more women. Maybe those could even rise further because of more balanced participation. An example is biomedical engineering, which in a lot of universities is a newer program, and ours is 50% men and women in terms of students and in terms of faculty as well.

But there are other fields that do well. Both in science and engineering, by increasing diversity and looking at equality, there are new things that are happening. For instance, just in the last couple of years at the University of Ottawa, there's been a lot around entrepreneurship and women in entrepreneurship, so I'll give you a couple of examples. We run a peer mentoring program with women entrepreneurs in the Faculty of Engineering. We've had a huge increase, starting from zero or one person to now a 50/50 split in terms of all of our competitions for entrepreneurship. But also, the types of things that they're coming up with as ideas for entrepreneurial ventures are increasingly associated with making a difference in society. We have students coming up with solutions to work with Syrian refugees who have arrived recently in Canada. We have a student who's looking at feedback devices for women's health problems and things like that. So, I think you will see change in both science and engineering as you include more women, and, if we can convince the people with the money or the power to invest in these areas, I think this is one major outcome.

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From schools, to universities, to a career in research, at what point do you think women are most underrepresented or struggling to progress in science and engineering?

Dr Tamara Franz-Odendaal: I think when we're talking about underrepresentation of women in science and engineering, we really can't lump all the subdisciplines in science and engineering in the same category. So, when we're looking at, for example, biology, we have no problem recruiting women into biology, but we still have a problem after they reach the PhD level to get into academia or industry. But when you're looking at engineering or computer science, there's a problem at the recruitment level into those programs.

If you have a problem at the recruitment level, you're going to have a problem when you are trying to hire women in these STEM programs because the pool is just that much smaller. So we really do need to use different strategies for the different subdisciplines within STEM. 'It's about providing opportunities for people to see themselves as leaders. If you want to have more diversity in leadership, you should give people from a diverse background or from all segments of the society opportunities.'







I think the point that is common among them all – where we really see a massive under-representation – is in leadership within STEM. We need to see a shift in the leadership so that we can do better hiring, use better hiring practices and better recruitment strategies and increase our talent pool when we are looking to hire women in STEM.

What specific measures do you think are required to increase gender equality and diversity within academia? How is NSERC working to achieve that?

Dr B. Mario Pinto: In order to have this balance, or any change in the ratios of faculty complements of under-represented groups, including women and indigenous peoples, one really has to begin with education of the current faculty complement – education in terms of conscious and unconscious bias.

This consists, first, of education in the value of diversity as I've just articulated, but then, second, of education in the principles and practice of conscious and unconscious bias. And it begins there. Although we train a great number of women in post-doctoral areas, for some reason, they are not hired at the same rate as their male counterparts, even though we attest to their excellence in research. So we feel that there is a bias, and it needs to be addressed at that initial phase of hiring – that's the first step. The next step, of course, is progression through the ranks, where it's a little bit more complicated, because there are different cultural pressures, and one has to take those into account.

You asked how NSERC is working to achieve this. We've realised, and others have too, that we have to recognise that women, for example, may have non-linear career paths. It's not all in lockstep like their male counterparts, and there may be gaps. There may be gaps for child-rearing, there may be gaps because they come from other career paths and so on. One really has to recognise that this is just a fact of life, and that one should take those differences into account. Assessment of a curriculum vitae then has to be done differently, because if one uses traditional measures, one will not arrive at the same conclusion about the quality of that candidate because, for example, there may be gaps in publications because of childrearing and so on.

What has NSERC done? Several things. First, we're making allowances for maternity leave. We extend grants automatically, but we start even further back with graduate students and postdoctoral fellows. We reassure them that they have paid parental leave if they are raising children or having children. It starts at that level. After they are hired as faculty, then we make sure that we extend their grants automatically and that they're given a chance to get back in the workforce full-time and keep producing at a scholarly level.

That's one of the things we're doing. The other is, we're educating our grant evaluators – we have many peer reviewers

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- in conscious and unconscious bias. And I think it begins there. Of course, these are all faculty members, and we're hoping that there will be multiplier effects as they go back to their universities and adopt our practices in those institutions because, as I said, it starts there. We have to get past this issue of conscious and unconscious bias and, in particular, how we evaluate individuals differently. They all have different circumstances, yet we have in the past been pretty uniform in how we assess candidates: numbers of publications and international presentations. That may not be the best way, as parents may not find it convenient to travel in the same way as people without children.

We are living in a very different world, where access to information is now freely available on the web. One has Skype and other modes of communication. Perhaps we should be re-examining the traditional measures of success. And I think that's really what it comes down to. We have to ask about impact and how we're measuring impact. Are the measures of impact correct? And I think we've come a long way. We have generated an equity framework at NSERC, and we have come up with a strategy to assure ourselves that we're giving all candidates the best possible chance when they are evaluated.

How can more diversity in leadership roles be promoted and future strong role models be supported?

Dr Tamara Franz-Odendaal: I think one of the clear messages we heard today at the Gender Summit was: if we use the same strategies, we're going to get the same results. We really need to change the way we've been doing things, and our Chief Science Advisor for Canada gave a great example today in her keynote speech, which was the example of how we view excellence in research.

Traditionally (in the past) and actually (right now), we use the number of international talks that a researcher has done as an indicator of research excellence, and that is not a familyfriendly policy or criterion. So that's one example of how using the same strategies is going to end up with the same result.

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Dr Annemieke Farenhorst: It's about providing opportunities for people to see themselves as leaders. If you want to have more diversity in leadership, you should give people from a diverse background or from all segments of society opportunities. And one of the things I can think about are leadership workshops for women, which, I think, are very, very important, so people can actually learn skills or advance their skills and feel more confident in being a leader.

Dr Catherine Mavriplis: Today at the Summit, we heard from Dr Elizabeth Cannon, and now we know more about the academic area in promoting leaders. She mentioned ELATE (Executive Leadership in Academic Technology and Engineering) as a program that trains leaders at Drexel University in engineering. This program comes from ELAM (Excellence Leadership in Academic Medicine at the Duke University School of Medicine), in which women can get some mentoring and training to step into leadership roles.

In our country, we've been told now by Minister of Science Kirsty Duncan that the universities won't get their funding

unless we meet diversity targets, so people are starting to mobilise there.

But Dr Cannon said it's important to make sure there are women who are already positioning themselves well for these leadership positions. It's up to the faculty, when they take these new leaders on, to make sure they're part of the team and that they're moving forward, to be able to do those things in the future.

How can the challenges of including other minorities and communities such as indigenous people and those with different gender identities start to be addressed?

Dr Annemieke Farenhorst: I guess there are two very different parts to that question. If I focus on the indigenous people, when I think about Canada, we certainly need more university graduates to meet the labour market demand, and indigenous people are the fastest-growing segment of Canadian society. So, for example, in the province where I live in – Manitoba – one in every five pre-schoolers are indigenous. It's the same in the neighbouring province of Saskatchewan.

We know that the indigenous population is fast-growing, but when it comes to university degrees, relatively speaking, a smaller proportion of indigenous people have a university degree compared to the non-indigenous Canadian population. So I think it is certainly important to be more inclusive. We are at the Gender Summit in Montreal, and one of the panellists today is Zabeen Hirji, who said something profound: 'Diversity is a fact, but inclusion is a choice'.

When we are thinking about inclusion, it should really be part of the strategic plan of organisations to actually make the workplace inclusive, whether we're talking about indigenous people, people of different genders, visible minorities and so forth. It really has to be supported at the top.

When I think about universities, there are a number of universities across Canada that have looked at indigenisation of their institutions – what that may mean and how that can be done. I think what is important within a university setting is the indigenisation of the curricula but also indigenous leadership in universities so students can actually see themselves. They can see the role models, and they can strive for something; they can also feel at home within the institution. So I think it's very important to look at curricula and expanding that as well as focusing on recruiting role models within universities or other organisations so that the young people can actually see themselves in those role models.

Overall, what do you see as the main challenges getting in the way of increasing diversity and inclusion in science and engineering? How do you hope Gender Summit 11 will contribute to facing these problems? 0

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Dr B. Mario Pinto: Let me start with Gender Summit 11. I think the most useful thing about all of these Summits is the conversations one has. One brings to the fore these critical questions; one asks hard questions; one shares best practices between different groups and different cultures; and, by sharing best practices, one takes those back to one's institution. Implementation of some of the best practices, for example, in Ireland, will lead us in the right direction to assuring greater gender equity in hiring practices. So that will increase diversity and inclusion in science and engineering.

The challenges, of course, are at the initial level, with those research peer review committees. One has to ensure diversity on those committees to begin with. It's going to take some time, because we can show clearly that inclusion of diverse groups leads to very different decision-making, and that includes decision-making with respect to hiring, with respect to choosing candidates for awards, etc. In the long-term, these small steps will lead to change, but it's going to take some time because it will take some turnover in the professoriate to complement these practices and adjust the gender balance.

Of course, the face of Canada is changing dramatically. Immigration is increasing. We're attracting foreign students, many of whom are staying and joining the workforce. Given that change in demographic, one would expect also a change in inclusion and diversity practices. But it will take time. There will be a lag time. But putting these policies in place and having open discussions in gender summits will get us all moving in the right direction together.

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THE AMERICAN SOCIETY OF MECHANICAL ENGINEERS

Founded in 1880, The American Society of Mechanical Engineers (ASME) is a non-profit organisation that facilitates collaboration, career development and upskilling across all engineering disciplines. Now representing more than 130,000 members in 151 countries, the Society's mission is to advance, disseminate and apply engineering knowledge to benefit people's lives and livelihoods. In this exclusive interview, we had the pleasure of speaking with Dr Charla Wise, ASME's President. Here, she discusses ASME's history, and how the Society achieves its goals through facilitating collaboration, influencing policy, recognising outstanding achievements and inspiring the next generation of engineers.



To begin, please tell us a little about the history of ASME.

This is such an exciting time for ASME! This year we are celebrating our 138th birthday and the Society is stronger than ever as we serve members and society well into our second century. One of the constants across all these years is our focus on safety. In the early years of our existence, ASME led the way in developing standards on boilers to end a significant danger to public safety of the time – the devastating and lethal explosions of steam boilers. Thanks to the early work of ASME, that public threat has now diminished.

The Society's founders were concerned citizens of that time, prominent machine builders and technical innovators of the late 19th century who saw how standardised design and production could increase safety and prosperity for everybody. Alexander Lyman Holley, one of the foremost steelmakers of the day, was one of our founders; so was Robert H. Thurston, the first professor of Mechanical Engineering at Stevens Institute of Technology. Thurston served as the Society's first president. We're also proud that Thomas Edison and Henry Ford were members of ASME in those early days too. The organisation they were a part of helped develop standardised tools, easily replaceable machine parts, and uniform work practices to ensure the reliability and safety of machines and industrial production.

What's the Society's mission, and how do you work towards realising it?

As president of today's ASME, I feel so fortunate to work with leaders and volunteers at all levels of a now modern, global organisation that supports ASME's continuing mission: to serve diverse global communities by advancing, disseminating and applying engineering knowledge to improve the quality of life and to keep our work going by communicating the excitement of engineering to inspire the next generation to join the effort.

We focus on making sure today's engineering workforce is well equipped to solve today's and tomorrow's technical challenges. We share with young people how rewarding it can be both professionally and personally to take part in creating solutions that truly benefit humankind.

What do you see as the most important areas of technological innovation for mechanical engineers now and in the future?

We live in an amazing time for engineers and technology professionals around the world – after all, the importance and impact of technology innovation are increasing each day in every area of modern life. Just think, 'Big Data', the 'Internet of Things' and artificial intelligence - the technologies of tomorrow are already here! But to answer your question specifically, ASME recently named five core technologies that we find central to engineers of today and tomorrow. They are: manufacturing (including advanced and additive technologies), pressure vessel technologies, clean energy, bioengineering, and robotics.

'As president of today's ASME, I feel so fortunate to work with leaders and volunteers at all levels of a now modern, global organisation that supports ASME's continuing mission'



The future is bright with innovation in every one of these areas of engineering. I get excited when I think of all the areas in which ASME is involved and the solutions our members have been a part of. Just think how engineers are creating and using drones to do safety inspections or building robotic exoskeletons to allow people who might never have walked again to do just that. Technologies like these and many more are already in use and will surely be improved, expanded, added to, and made more easily accessible to more people with each passing day and year. Think about it: if 'it' is a machine and 'it' moves, mechanical engineers have a role to play in its future!

Please tell us a bit about the resources you provide that can enhance and develop your members' careers and promote collaboration.

Becoming a part of globally-recognised and respected community of professionals is empowering to each individual involved. ASME has a vast and diverse membership of 110,000 mechanical engineers and tech professionals from around the world. ASME offers tools, events, programs and publications, just to name a few, to enable collaboration and technical cooperation with the world's most distinguished and recognised engineers.

Our community is a global network that connects members in so many regions, working together in every area of the Society, including codes and standards development, continuing engineering education, research, professional conferences, peerreviewed publications, public policy and advocacy. These are just some of the topics within the amazing range of disciplines that ASME addresses on a daily basis. ASME offers so much professional community, resources, deep subject-matter expertise in every engineering discipline, opportunities for learning, service, professional development and fellowship and a chance to serve a worthy mission in a community devoted to excellence.

As an example, one of ASME's chief aims is to help the next generation of engineers find their professional way forward. To do this, we offer our 32,000 student members an array of opportunities for career preparation. One new and very exciting program we launched in 2017 is called E-Fests. E-Fests are regional events held at universities around the world that provide engineering students a chance to come together, showcase their skills and abilities through various design competitions, learn from professionals and from one another, and to have a great time. E-Fests are true Engineering Festivals as their name implies. You can see a video at https://efests.asme.org/.

ASME also produces a wide range of programs for engineers who are already in the workforce. ASME's Learning & Development area offers both online and classroom-style training pertaining to many of ASME's more than 500 codes and standards. Classes scheduled in 2018 will cover piping, pressure vessels, and verification and validation. This means that the ASME Code, the best and most reliable engineering code in the world, also comes with extensive training in how to make sure engineers are using it in the most skilful way possible. 'Standards may not always be considered 'glamorous', but there's no denying that strong and reliable standards are foundational to the health of the world economy'



Another wonderful new program is based on the amazing developments, growth, and interdisciplinary nature of the biomedical engineering field. ASME is 'parenting' a new professional organisation called the Alliance for Advanced Biomedical Engineering (AABME) <u>https://aabme.asme.org/categories/wearables-embedded-bioprinted-sensors</u>. The AABME brings together a broad interdisciplinary community of technical professionals to catalyse the development of life-enhancing applications in the areas of tissue engineering, organ manufacturing, and cell therapy.

We are so proud of all these efforts. And we're just scratching the surface here!

Does ASME advise the US Government on engineering related policy?

ASME has a Government Relations (GR) team, which is recognised throughout Washington for its outstanding capabilities! The GR Team is sought out to lead policy related issues by policymakers as well as fellow Associations and industries. ASME's Government Relations team, which consists of staff and volunteers, offers policymakers access to technical expertise, knowledge and advice to help them make the decisions that affect everyone. This work includes the creation of formal position statements and white papers to support US federal investment in the work of the nation's science and technology agencies, congressional visits, and convening forums and events in Washington, D.C. for the engineering community.

We also work closely with distinguished ASME members from industry and academia to provide briefings to Congressional staffers as a way to keep them current with the technical public policy issues currently under consideration in Congress. For example, two recent briefings focused on 'Connected & Autonomous Vehicles: Incorporating AVs into our Transportation Infrastructure' and 'Department of Defense's New Manufacturing Engineering Education Grant Program'.

One of the longstanding ways ASME helps advise policymakers is through the ASME Federal Government Fellowship Program. This program was established in 1973 and selects highly accomplished ASME members to serve a year working in the Congress or the Executive Branch to provide objective, non-partisan engineering expertise to US policymakers. ASME has sponsored 120 Federal Fellows over the past 44 years. We're very proud of the ASME Federal Fellows program and its continuing commitment to provide engineering expertise to government. It's a great and unique opportunity for an engineer to grow as well.

Tell us about ASME's awards to recognise outstanding achievements in mechanical engineering?

ASME offers hundreds of awards and scholarships to recognise and celebrate the extraordinary achievements of engineers! We believe that recognising these outstanding achievements and contributions of our professionals and students serves two purposes: it disseminates and spreads knowledge for the advancement of engineering and technical solutions and it serves to inspire professionals and to excite our engineers of the future!

ASME presents many different awards every year to recognise distinguished achievement in and contributions to engineering as well as dedicated service to the Society itself. The highest award bestowed is the ASME Medal. Established in 1920, the ASME Medal is given annually to recognise exceptionally distinguished achievement and contributions by an engineer over the course of his or her full career. The list of ASME Medal recipients includes renowned figures such as Igor Sikorsky, Dean Kamen, and Norman Augustine. The 2017 ASME Medallist was Professor Zdeněk P. Bažant of Northwestern University, recognised for his singular contributions to the probabilistic theory of materials and structures. A world-leading scholar and the author of seven books, we thank Dr Bažant for increased safety in bridges, dams, buildings, aircraft, ships and nuclear containments.

Tell us about some of your upcoming conferences. In what ways do these meetings promote innovation?

Over 25 conferences and hundreds of committee meetings are planned in 2018 at the national, international and local levels. The Society is offering a full schedule of technical conferences around the world including Turbo Expo, to be held in Oslo (Norway) in June; ASME's Power & Energy Conference in Orlando, FL (USA), also in June; the Pressure Vessels & Piping Conference in Prague (Czech Republic) in July, and the Nano Engineering for Medicine and Biology Conference (NEMB) in Anaheim, CA in August. Our biggest conference of the year, the International Mechanical Engineering Congress and Exposition (IMECE), will be held in Pittsburgh, PA in November. IMECE offers the broadest range of technical sessions, with topics from aerospace and energy to materials science to medical devices all happening over the course of a week.

ASME conferences bring together thought leaders, academics, and leading practitioners from every corner of the globe to discuss the very latest advances in technology and new product applications, to meet, talk, network, connect, and collaborate. These gatherings are some of the world's largest gatherings of mechanical engineering expertise in every area and naturally serve as essential vehicles for communication and information exchange.



Please describe the Society's role in developing codes of practice and standards for the mechanical engineering industry. Why is this work still so important?

ASME is recognised worldwide for developing and producing some of the most detailed, accurate and consensus-built standards in the world! Codes and standards have played a central role in the Society's history and growth. In its early years, ASME led the way in this activity, creating standards for screw threads, pump and valve dimensions, and other mechanical components needed to empower the rising productivity of factories, machine works, and even farms. In 1914, a major milestone in Society history occurred with publication of the first edition of the ASME Boiler and Pressure Vessel Code: Rules for the Construction of Stationary Boilers and for Allowable Working Pressures. Ever since then, professionals have come together to develop engineering standards for use in many technical areas including



pipeline production, elevators and escalators, cranes and other lifting devices, gas turbines, and commercial nuclear power.

Why is this work still so vital? Standards are indispensable to modern industries of every kind – they allow safe and uniform design approaches in engineered systems, which is what makes those systems reliable, interoperable, and safe. As engineering continues to cross borders and manufacturers establish operations across the globe, widely accepted standards are critical to making products manufactured in one part of the world safe and useful in markets in other parts of the world. Standards may not always be considered 'glamorous', but there's no denying that strong and reliable standards are foundational to the health of the world economy.

What is the ASME Foundation, and how does it support young engineers in their education and career development?

The ASME Foundation Goal's is to move the needle forward and make a difference in inspiring current and next generation engineers! The ASME Foundation does wonderful work on behalf of the mechanical engineering profession, including sponsoring and supporting programs in STEM education and career development and providing scholarships.

One program made possible by the ASME Foundation is *Future Engineers*, a STEM education program that ASME has now produced for several years in collaboration with NASA. *Future Engineers* challenges have included a contest in which K-12 students were asked to dream up and design objects for 3D printing on the International Space Station and then for use by real astronauts.

A second very popular and quite ambitious initiative of The ASME Foundation is the ISHOW (short for *Innovation Showcase*), in which young engineer-entrepreneurs working on hardware projects to support sustainable development can enter their designs in three different global competitions to earn seed money and how-to advice from professional firms to help their start-up enterprises succeed.

Finally, what do you see as the biggest challenges facing mechanical engineers in the next ten years? How will ASME support its members to tackle these challenges?

One of the biggest challenges we will have is educating and training sufficient numbers of engineers to help create the future and solve upcoming technical challenges. Our increasingly data-driven world economy is putting a premium on engineers' ability to create sophisticated computer code and develop algorithms to allow companies to manage their supply chains, internal operations, product development timetables, and other essential business functions. We need to help more engineers master those particular challenges.

Another major task engineers must tackle is maintaining the safety and reliability of the advanced technologies flooding the marketplace: autonomous robots, self-driving cars and trucks, and 3D-based product fabrication. These are all important new areas of the economy and they will all surely mature over time. In the case of 3D fabrication, for example, while it is an amazing boon to aerospace and automotive companies to be able to 3D-print needed components on demand, we still need standards of quality control, rigor and oversight to insure the

'When it comes to bringing the benefits of technology to the world and helping the amazing engineering and technology professionals who are doing it, ASME will be right there with them making it happen'



safety of those components. ASME standards-creators have begun to address this need, for example in our December 2017 publication of *Product Definition for Additive Manufacturing*, which applies to parts and assemblies designed in additive manufacturing environments.

Another challenge for engineers – as well as policymakers – is finding practical and cost-effective technical solutions to the global problems of water management, energy supply, and health assessment. ASME's aforementioned ISHOW brings engineers to the forefront of addressing those challenges, with three global competitions each year showcasing products and systems created to help developing countries around the world. Another emerging industry trend is the growth of advanced and additive manufacturing techniques. There are many new and unmet needs in the additive manufacturing space, particularly in the area of materials characterisation.

As we move into the future, ASME will continue to assess the changing world environment of the engineer and organise specialised conferences, workshops, and other forums to help our members gain a competitive edge. When it comes to bringing the benefits of technology to the world and helping the amazing engineering and technology professionals who are doing it, ASME will be right there with them making it happen. We are helping to create the future, safely!

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ENERGY

COMBATING CLIMATE CHANGE WITH CLEAN ENERGY TECHNOLOGIES

Our insatiable demand for energy has pushed the planet to the brink of disaster. Because of the widespread use of fossil fuels as our primary energy source, coupled with extensive deforestation, levels of carbon dioxide and other greenhouse gases in the atmosphere are at an all-time high.

In fact, compared to pre-industrial times, the concentration of carbon dioxide in the Earth's atmosphere has risen by a whopping 45% – almost entirely due to human activity - up to its current value of about 406 ppm (October 2018). This, combined with increases in other anthropogenic greenhouses gages, such as methane, has led to an average temperature rise of 1.1°C, with much of this increase attributed to the last few decades. Worryingly, at the time of writing, 17 of the 18 hottest years on record have occurred since just 2001. This warming is a major culprit behind the increasing prevalence and severity of storms, droughts, wildfires and floods that we are currently experiencing.

Earlier this month, the UN issued their landmark climate change report, which warns of the imminent threat to the planet before 2040 if drastic measures are not implemented within the next 12 years. The report urges that global warming must not surpass a maximum of 1.5°C (just 0.4°C above the current temperature). Even half a degree more than this limit will significantly worsen the risks of flooding, extreme heat, drought, famine and poverty for hundreds of millions of people worldwide.

The UN report finds that Earth's wildlife will suffer most if this 1.5°C limit is surpassed. For example, insects are twice as likely to lose half their habitat at 2°C of warming compared with 1.5°C. Such a scenario would have an utterly devastating impact on our food supplies, as many of our crops are reliant on insect pollination.

Therefore, a complete switch to lowcarbon energy, such as that generated by wind farms, hydroelectric stations, solar farms and nuclear power plants, needs to happen as soon as possible. To facilitate this urgent shift, thousands of engineers and scientists around the world are developing more effective, affordable and safe renewable energy technologies. Many are also finding novel ways that we can conserve energy, particularly in industrial processes, while others are working to develop better means of storing energy. In this section, we feature a number of promising research projects in these areas.

To introduce this section, we have had the pleasure of speaking with Dr C. D. Mote, Jr, president of the US National Academy of Engineering (NAE). In this exclusive interview, we discuss the NAE's 'Grand Challenges for Engineering' program, which aims to inspire young engineers to address humanity's greatest challenges, with a particular emphasis on developing affordable renewable energy technologies.

Marine energy technologies comprise one group of underutilised renewable energy devices. Such technologies include marine hydrokinetic devices, which harness the energy of moving water, and offshore wind turbines. However, the viability of these technologies and their potential environmental impacts need to be better established, before they can be widely implemented. In this section of the edition, we meet Dr Grace Chang and Dr Craig Jones from Integral Consulting Incorporated, who are working towards this goal. Their research will inform and expedite the environmentally responsible implementation of these technologies.

Next, we introduce the research of Dr Wei-Chau Xie of the University of Waterloo, whose aim is to improve the safety of another source of low-carbon energy – nuclear fission. Although nuclear power plants are some of the most secure structures in our society, when subjected to earthquakes, they have the potential to cause major disasters. Dr Xie and his research team develop algorithms to test the safety



of these structures – analysing their properties as they are subjected to seismic activity. Their research has provided new insights into how nuclear power plants may be designed to withstand stresses resulting from earthquakes, protecting nearby populations.

In our next article of this section, we meet Dr Saniya LeBlanc and her research team at the George Washington University, who devote their time to developing thermoelectric generators, which turn heat directly into electricity. During countless processes, such as driving a car, using a laptop and manufacturing glass, energy is wasted as heat. The team's devices could be used to convert this wasted heat into electricity, which could be pumped back into the system, making the process far more energy efficient.

One particular process that uses enormous amounts of energy is the Haber-Bosch Process, which converts nitrogen into ammonia on an industrial scale. Used to create a whopping 450 million tons of agricultural fertiliser every year, this process accounts for approximately 2% of the total energy expenditure of the entire world. Therefore, many researchers are looking for alternatives.

In the next article of this section, we meet Dr Douglas Way and Dr Colin Wolden, who are collaborating on a project that could not only improve the energy efficiency of ammonia production, but also provide a means of reducing carbon dioxide emissions throughout the entire industrial world.

From here, we move on to showcase research into safe, affordable and efficient energy storage devices. Such energy storage is critical to the functioning of many renewable energy technologies. For example, without energy storage, excess solar energy that is captured by photovoltaic cells during the day would be wasted. With energy storage, that energy can be stored and used later, especially at times when sunlight is unavailable.

First, we take a look at lithium battery research. Here, we introduce Dr Partha Mukherjee and his team at Purdue University, who are gaining deep insight into the complex interactions that happen inside lithium-ion and lithium-sulphur batteries. Through these investigations, the team's ultimate goal is to improve the performance and safety of these devices.

Then, we move on to different type of energy storage device – the capacitor. In the final article of our energy section, we showcase the work of Mr John Fraley and his colleagues at Wolfspeed and International Femtoscience. This interdisciplinary team of engineers and scientists is working on a new generation of capacitors, which show greatly improved energy storage capabilities over our current technologies.

THE US NATIONAL ACADEMY OF ENGINEERING









Founded in 1964, the US National Academy of Engineering (NAE) is a private, independent, non-profit institution that provides engineering leadership in service to the nation. It has a long and illustrious history serving the American people in its role to advise and support scientific and engineering advancement both in the US and world-wide.

In this exclusive interview, we talk to the NAE's president Dr C.D. Mote, Jr. about the NAE and its 'Grand Challenges for Engineering.' This program is aimed at inspiring young engineers across the globe to address the biggest challenges facing humanity in the 21st Century. From the need to develop affordable clean energy solutions and increase access to renewable environmental resources, to facing new challenges in healthcare, these challenges potentially impact on the quality of all our lives. These global grand challenges are huge in scope and address the biggest current concerns of all the world's citizens. 'The Grand Challenges for Engineering project was conceived to raise public awareness – especially among young people – of some of the biggest global issues of our time and the roles that engineers, and engineering must play in addressing them.'



To begin, can you please tell us briefly about the National Academy of Engineering and its role in promoting engineering and providing leadership for the engineering community in the US?

The mission of the National Academy of Engineering is to provide independent, trusted advice to any department of the federal government to advance the well-being of the nation and to promote a vibrant engineering profession. This is accomplished by marshalling the expertise and counsel of eminent engineers.

The NAE has more than 2,000 peerelected members and foreign members, senior professionals in business, academia, and government who are among the world's most accomplished engineers. They provide the leadership and expertise for wide-ranging projects serving the needs of people and society.

The NAE is one of The National Academies of Sciences, Engineering, and Medicine. The three academies operate in the same building under the same congressional act of incorporation that established the National Academy of Sciences in 1863 by President Lincoln. Under this charter the NAE is directed, 'whenever called upon by any department or agency of the government, to investigate, examine, experiment, and report upon any subject of science or art,' where 'art' includes all human creations.

Can you tell us a bit about the origins and purpose of the NAE's grand challenges for the future of engineering?

The Grand Challenges for Engineering project was conceived to raise public awareness – especially among young people – of some of the biggest global issues of our time and the roles that engineers, and engineering must play in addressing them.

The project, funded by the US National Science Foundation, convened an international committee of some of this generation's leading technological thinkers and doers. With wide-ranging voluntary inputs on what engineering should contribute in the 21st century from people in more than 40 countries, ranging from engineering experts to the general public, the committee identified a 21st century engineering vision for the planet focusing on the needs of people. The committee's report, released in 2008, identified its 15-word vision for engineering in the 21st century as the 'continuation of life on the planet, making our world more sustainable, secure, healthy, and joyful.'

The report also presented 14 goals that must be satisfied globally to realise this vision. Those 14 goals are named the Grand Challenges for Engineering. Satisfying these grand challenges everywhere is necessary to realise the vision and improve quality of life here on Earth.

The Grand Challenges for Engineering are global-scale engineering system challenges whose solutions will depend on contributions from around the world. The grand challenges are arguably the



clearest and most compelling explanation of what engineering is for students and the public alike because they illustrate both the vast span of the field of engineering and how engineering serves people and society, both not generally understood. This is the first global vision for engineering in history.

Can you give a brief summary of some of these challenges and how addressing them will impact on quality of life across the globe?

The Grand Challenges for Engineering are as follows. To make solar energy economical, to develop carbon sequestration methods, to manage the nitrogen cycle and to provide access to clean water. They also include developing enhanced virtual reality, advanced health informatics, restoring and improving urban infrastructure and engineering better medicines. As well as preventing nuclear terror, securing cyberspace, reverseengineering the brain, advancing personalised learning, engineering the tools of scientific discovery and providing energy from fusion.

Our planet's very survival, as we know it, depends on satisfying many of these challenges. In addition, the vision, underpinned by the Grand Challenges is the first engineering vision that mandates global perspective. The vision cannot be realised by a few nations, though a few nations can inspire attention to it. Each grand challenge needs to be achieved in all global locales and circumstances.

For instance, the challenge to 'provide access to clean water' is for everyone, those alive today, including those with contaminated water and those with no water at all and those yet to be born in this century. Each challenge is to be fulfilled globally by assembling solutions as needed locally. Because the vision is about life for all, this is a rare circumstance where people everywhere, across diverse cultures and countries, share in the importance of the Grand Challenges. There are no losers in this vision.

Since their publication in 2008, the Grand Challenges have spawned a biannual series of Global Grand Challenges Summits and a Grand Challenges Scholars Program that prepare students and the public to address these challenges and engineering system problems like them.

How are you supporting the education and training of the next generation of engineers? For example, can you tell us about the NAE Grand Challenges Scholars Program?

Because the vision for the Grand Challenges for Engineering and their solutions are global, fulfilling that vision requires engaging people all over the world. Given the interest young engineers everywhere have expressed in these challenges, including their participation in our three global summits (detailed later) and engaging them in the Grand Challenges Scholars Program (GCSP) has inspired young people to work on the challenges globally.

This is a principal goal of the GCSP and is the key to achieving the vision of the Grand Challenges for Engineering. A second, broader goal is to prepare students for the multicultural, multidisciplinary, socially conscious global engagement needed for 21st century engineering in general. The Grand Challenges Scholars Program is an engineering program supplement that is implementable in any existing university engineering program without disrupting its program.

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'Grand Challenges for Engineering are not US grand challenges but are global grand challenges whose solution serves all people so international engagement is necessary. This is a first in history.'



The Grand Challenges Scholars Program was introduced in 2009, just one year after the Grand Challenges for Engineering report was published. Its singular role is to enhance students' competencies in five areas that are not commonly found in engineering curricula.

Research/creativity

Mentored research or creative experience on a Grand Challenge-like topic; *talent competency*

Multicultural understanding

Understanding of cultures, preferably through a multicultural experience, to ensure cultural acceptance of proposed solutions where they are implemented; *cultural competency*

Multidisciplinarity

Understanding of multidisciplinary engineering system solutions, developed through engagement; *multidisciplinarity competency*

• Viable business/entrepreneurship Understanding, preferably developed through experience, of the necessity of a viable business model for where a solution is implemented; *business competency*

Social consciousness

Understanding that solutions should serve primarily people and society, reflecting social consciousness; service learning promotes social consciousness; *social consciousness competency*

In creating a Grand Challenges Scholars Program, two questions were of primary importance. For the students, what supplement to a traditional engineering program would stimulate their interest in and preparation for the vision and goals of the Grand Challenges for Engineering and problems like them?

For the universities, what supplement could be easily implemented everywhere on the planet to prepare students for global engineering initiatives that concentrate on the highly valued program outcomes (the five student competencies) while leaving all program operations to each university?

Each university selects its students, educates its students on the five competencies, evaluates student achievement on them, determines those students who merit recognition as Grand Challenges Scholars, and recognises them appropriately. Each university operates its own GCSP

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independently of all others, other than accepting the responsibility to educate its students on the five student competencies. The GCSP addresses the needs of both students and universities beautifully.

In 2017 more than 100 US engineering colleges have a Grand Challenges Scholars Program in operation or under development. The US's goal is to expand to 200 Grand Challenges Scholars Programs, which will include about half of the engineering colleges in the country. Seven international engineering colleges have operating Grand Challenges Scholar Programs while more than twenty additional colleges are developing programs.

The international goal is to expand to 200 Grand Challenges Scholars Programs abroad. Interest in the program among students is high, so continued growth, often driven by the students themselves, is realistic. Furthermore, the GCSP is attracting students from diverse backgrounds, especially women and underrepresented minorities, who constitute more than half of the students in the program, although they account for about a quarter of the US engineering student population.

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Participation in the program by students from fields outside engineering is also common and determined by each university.

Finally, I would note that the Grand Challenges for Engineering are also being incorporated in community colleges and in K-12 school programs across the US, both within their curricula and in after school activities.

How are you encouraging international collaboration to address these global challenges? Can you tell us a bit about the Vest Scholars Program and the Global Grand Challenges Summits?

Let me start with the Global Summit series. The Global Grand Challenges Summits have been hosted jointly by the NAE, the UK Royal Academy of Engineering, and the Chinese Academy of Engineering beginning in London in 2013, the next in China in 2015, and the most recent was in Washington, DC in 2017. The summit series facilitates collaborations to address the Grand Challenges, maintains the focus on the Grand Challenges vision, and, importantly, is an opportunity to inspire students and next-generation engineers to engage with the Grand Challenges for Engineering.

The latest event in DC was the largest program in NAE history, with some 900 attendees, more than half of whom were university students from 150 universities across the three countries. It required multiple venues at the National Academy of Sciences building, George Washington University and the US Institute of Peace. The thematic foci were sustainability, health, security, and joy of living, as well as education and public engagement. Topics included virtual reality and artificial intelligence, engineering and healthcare, climate change, and reverse engineering of the brain.

The program was divided between expert presentations on the progress made toward addressing the Grand Challenges and the dynamic ways to engage student interest and participation. For the students, there were poster and business plan competitions, a podcast competition on, 'How to Change the World', and extended Q&A opportunities with the speakers and sponsors. Student presentations on their experiences in the Grand Challenges Scholars Program highlighted the transformational impacts of this program on their education and, the highest accolade of all, on their choice of an engineering career.

In addition, in a collaborative arrangement with NAE member Dean Kamen, the inaugural FIRST Global Challenge robotics competition -FIRST stands for, 'For Inspiration and Recognition of Science and Technology' - drew high school student robotics teams representing 157 countries in an Olympic Games style team competition held in conjunction with the global summit. The contest asked participants to take on one of the Grand Challenges - providing access to clean water. The Charles M. Vest NAE Grand Challenges for Engineering International Scholarship Program - The Vest Scholarships – was launched in March 2013 at the inaugural Global Grand Challenges Summit. This program provides opportunities for graduate students at selected international universities to pursue research addressing a global Grand Challenge at a leading United States university, with expenses paid for a year of travel and study.

Finally, what do you see as key to the future success of tackling these Grand Challenges in the next ten years?

A necessary condition for achieving the vision of the Grand Challenges for Engineering is the successful global implementation of the Grand Challenges Scholars Program.

This conclusion is driven by the following observations. Students in the Grand Challenges Scholars Program are



highly committed to and excited about the Grand Challenges for Engineering. These students also have the capability to introduce the Grand Challenges for Engineering movement into their countries and local communities which otherwise would likely have no contact with it. They also have the potential for leadership to 'carry the banner forward' subsequently as they become professionals and volunteers.

The solutions to the Grand Challenges for Engineering are mandated to serve all global communities. After a decade following 2008, no viable alternative to inspiring international students for fulfilling that mandate is apparent.

Additionally, we need to further engage younger students – and their parents – by introducing them to the Grand Challenges for Engineering in and out of school and to raise awareness of them among media, policy makers and the general public.

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From the beginning, we recognised that the Grand Challenges for Engineering are not US grand challenges but are global grand challenges whose solution serves all people so international engagement is necessary. This is a first in history.



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TOWARDS LOW-COST, LOW-IMPACT MARINE RENEWABLE ENERGY

As we move towards a sustainable future, there is a growing interest in marine renewable energy technologies such as marine hydrokinetic devices and offshore wind turbines. However, the viability of these technologies and the potential environmental effects associated with their implementation needs to be established. Scientists **Dr Craig Jones** and **Dr Grace Chang,** from Integral Consulting Incorporated, USA, are working towards this goal.



Establishing the Viability of Sustainable Energy Technologies

The Earth is currently undergoing significant environmental and climatic change, and the negative impacts of our collective behaviour and lifestyle choices are becoming more apparent. Indeed, recent developments and unfolding ecological crises have highlighted the need to reassess the way we source and use energy. Therefore, sustainable and environmentally friendly energy resources and technologies are of primary concern to scientists and engineers around the globe.

One such area of technology development is in marine hydrokinetic energy, which harnesses the energy of moving water. Wave energy converters (WECs) and current energy converters, for example, are types of marine hydrokinetic energy devices that capture the kinetic energy of waves and tides and currents, respectively. Another marine renewable energy technology is offshore wind generation systems. Energy from these technologies is cleanly converted into electricity, which can be fed into the grid for the benefit of citizens.

However, each technology brings with it a whole new set of challenges. For example, the potential environmental effects associated with installation, maintenance and operation of WECs need to be established, as do the economic impacts. Gathering this information is crucial in ascertaining whether this technology is truly viable.

In fact, one of the first pilot-scale WEC deployment programs in the US was deemed unviable due to the costs and delays associated with acquiring permission to put the devices in the water. Subsequently, it was identified that the processes surrounding WEC implementation, and the management of environmental concerns, needed to be streamlined so that regulators



would be more confident that the technology is indeed a suitable, low-impact solution.

Physical and biogeochemical oceanographer Dr Grace Chang, and ocean and environmental engineer Dr Craig Jones, of Integral Consulting Incorporated have teamed up to tackle this challenge - bringing together their knowledge, insight and expertise. The team, comprising Integral Consulting Incorporated and Sandia National Laboratories, is supported by the US Department of Energy Office of Energy Efficiency and Renewable Energy (US DOE EERE) to research the potential effects of marine renewable energy technologies on the environment; specifically, on the ocean floor and coastal landscapes. This research can then inform and expedite the environmentally responsible implementation of these technologies.

The Effect of WECs on Wave Propagation

In a research project started in 2009, Dr Chang and Dr Jones aimed to understand the effects of WECs on nearshore wave propagation. In other words, their goal was to determine whether WEC devices would have a significant impact on the size of waves 'Our mission is to quantify the potential environmental risks of WEC deployments and reduce the time and costs associated with the environmental permitting process. We will engage with regulators and developers to participate in hands-on tutorials to learn the tools and techniques developed to understand the potential environmental effects of marine energy generation.'



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travelling towards the shoreline. This understanding is vital, as large arrays of WEC devices have the potential to adversely affect the local environment by altering normal circulation patterns, sediment mobility, and other ecosystem processes.

For this project, the team used a modified version of a standard wave model to simulate wave propagation through a hypothetical WEC array deployment of ten devices on the Californian coast. They simulated a number of realistic experimental conditions derived from real-world wave measurements in the model domain and made detailed comparisons between model results for 'average' (northwesterly waves) and 'south-swell' conditions. WEC effects were quantified by looking at wave parameters with and without devices deployed in the wave simulation zone.

The team found that the presence of the ten WECs had little to no effect on the height of waves under average conditions. While they found that wave height decreased by approximately 30% in south-swell conditions, the effects decreased substantially towards the shoreline to approximately 5%. The results indicated that WEC deployment does have the potential to affect natural processes, but potential impacts to the local ecology needed to be evaluated.

Dr Chang and Dr Jones then re-visited this experimental design in 2015. This time, they investigated the near- and far-field effects of device size and deployment layout patterns on wave propagation. The team found that, depending on the type of WEC, large arrays WECs did indeed influence wave propagation to varying degrees. However, the question still remained as to what effect these changes in wave propagation could have on coastal structures, processes and ecosystems, and whether it is a cause for concern.

Effects of WEC Systems on Marine Habitats

Ecological systems are sensitive to change in the physical environment. Therefore, changes in wave propagation could have a significant effect on local environments near the WEC deployment zone. For example, changes in the way waves move and distribute sediments may alter seafloor habitats. Changes in currents and circulation patterns have the potential to affect water quality and thus the behaviour of marine species.

Dr Jones and his team set up another case study in Newport, Oregon – a site that has supported and will continue to support WEC deployments. In this case study, the 18 WECs were laid out in a 50 m x 50 m grid, and the team's focus was on the effect on wave propagation during a moderate southerly swell and a moderate western wave event. The research team obtained the best available seafloor and ocean depth data at the test site from Oregon State University for comparative purposes.

Dr Jones and his team found that, as explained in their research paper, 'the alterations of wave heights, orbital velocities at the bed, and radiation shear stress in the lee of a WEC deployment do exhibit changes that could result in an environmental stressor.' However, to establish the true environmental impact of these changes, the data would need to be compared with datasets collected by other scientists assessing other physical and biotic parameters. For example, data on mid-water trawl fishing near the Newport site are readily available. A comparison of data sets could be used to ascertain whether the changes in wave propagation, circulation, sediment transport, and water quality affect the population densities of certain fish. However, initial results of these and similar studies show negligible environmental impacts for the small pilot scale WEC deployments.



Effects of Offshore Wind Infrastructure on Ocean Sediments

According to research by Dr Jones and his team, 'the offshore wind energy market has made large strides globally and is presently proving its viability. As the technology improves and the ability to deploy offshore wind turbines in deeper waters becomes increasingly feasible, developers and the government are continuing to find ways to expand the offshore wind market.'

However, there are challenges associated with offshore wind systems, which ultimately influence implementation cost and viability. One of these is in regard to the installation process, as it requires seafloor foundations, cabling, floating structures with gravity anchors, or a combination of several of these systems. The installation and presence of these structures may affect the integrity of the sediment bed or the way in which sediments are transported and deposited in near-shore coastal regions. This could have a significant impact on the local environment and ecosystems. So, in addition to the costs associated with construction, there is significant expenditure associated with acquiring permission from governmental authorities to build the systems.

In work funded by Sandia National Laboratories and the US DOE EERE, Dr Jones and colleagues from Integral Consulting carried out a study that examined the effects of offshore wind sub-sea foundations and cables on sediment transport. Their study also evaluated the potential risks associated with these alterations. Specifically, Dr Jones and his team developed modelling tools and techniques for developing maps indicating potential changes in seabed stability after the installation of offshore wind infrastructure. In summary, Dr Jones found that the presence of offshore wind structures reduces the sediment transport in the sheltered area of the deployment zone by altering current and wave fields. In a sense, this was no surprise to Dr Jones – he had observed a similar effect in his study of the impact of WECs on wave propagation. However, the methods for developing maps that the team produced, which outline the potential seafloor erosion, or scouring zones, provide developers with valuable planning, design, and evaluation tools for the siting and development of offshore wind power systems.

Informing and Training Regulators and Developers

Dr Chang and Dr Jones want to use their research to inform regulators and train developers who are involved with the design and implementation of marine renewable energy systems. When asked about their future work, Dr Chang commented: 'we will engage with regulators and developers to participate in hands-on tutorials to learn the tools and techniques developed to understand the potential environmental effects of marine energy generation.'

Of course, the work of Dr Chang and Dr Jones aims to preserve and protect the environment as best as possible, whilst utilising the abundant potential of marine renewable energy systems. And they also seek to improve the efficiency of the installation and construction process. As humankind pushes towards a more sustainable future, their work is certainly of great assistance in improving sustainable energy technology and reaching our renewable energy targets.





Meet the researchers

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Dr Grace Chang received her PhD in Marine Science from the University of California, Santa Barbara, in 1999. Her research pursuits have been in the fields of hydrodynamics, sediment transport, particle dynamics, and marine and hydrokinetic energy. She has managed programs involving field operations, data processing and analysis, numerical modelling for environmental characterisation, observational monitoring, scientific research, and the development of various technologies. She now serves as a Senior Consultant at Integral Consulting Incorporated and has more than 20 years of experience in long-term ocean monitoring and site assessments.

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Dr Craig Jones received his PhD in Mechanical and Environmental Engineering from the University of California, Santa Barbara, in 2000. He has since been involved in several research projects in the fields of riverine, lacustrine, estuarine and coastal hydrodynamics, wave propagation and sediment transport. He is skilled in the predictive modelling of physical processes involving extreme events, change analysis, and environmental risk assessment. He currently serves as principal ocean and environmental engineer at Integral Consulting Incorporated and has 20 years of experience in developing study programs for government agencies and the private sector for the characterisation of marine sites.

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SHAKING UP THE PHYSICS OF VIBRATION

Nuclear power plants may be some of the most secure structures in our society, but when subjected to earthquakes, they have the potential to cause major disasters. Dr Wei-Chau Xie of the University of Waterloo in Ontario, Canada, is now developing algorithms for testing computer models of these structures - analysing their properties as they are subjected to virtual seismic activity. His research has provided new insights into how nuclear power plants may be designed to withstand stresses resulting from earthquakes, protecting nearby populations.

Safeguards Against Disaster

When considering the issue of seismic activity, designers of nuclear power plants have needed to develop robust safety standards to prevent disasters from happening. Nuclear facilities around the world are designed to withstand earthquakes, and to shut down automatically during major events, in order to protect nearby populations and the environment.

Different countries have various safety standards associated with the analysis, design and construction of nuclear power plants. In France, where 75% of the country's electricity is generated from nuclear power, reactors are designed to withstand twice the force of the strongest earthquake expected to occur over 1,000 years for a given location.

Despite these precautions, disasters can still happen. For instance, on March 11th, 2011, the Great East Japan Earthquake, Tohoku, struck the island nation with a force measured at 9.0 on the moment magnitude scale. 11 nuclear power plants were shut down

automatically following the earthquake. Unfortunately, 15-metre-high tsunami wave flooded the Fukushima nuclear power plants, resulting in severe damage in three units, meltdowns, and the release of radioactive materials into the environment.

These events have prompted governments, nuclear regulatory groups, and researcher teams across the globe to take a new look at how nuclear power plants are protected from forces of the natural world.

Dr Wei-Chau Xie and his colleagues at the University of Waterloo in Ontario, Canada, are one such team of researchers. They are currently studying how nuclear power plants and other critical infrastructures and facilities can be protected from earthquakes and other natural disasters. Dr Xie's team employs a wide range of scientific disciplines in order to develop accurate estimates of different seismic hazards.

'The objective of our research is to have a better understanding of the dynamic and stability behaviour of structures and to provide methods for the reliability



and safety analysis and design of structures, machinery, and engineering systems in general,' Dr Xie explains.

Dr Xie and his colleagues are particularly interested in maintaining the safety of nuclear power plants. They conduct seismic risk analyses for various

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'The objective of our research is to have a better understanding of the dynamic and stability behaviour of structures, and to provide methods for the reliability and safety analysis and design of structures, machinery, and engineering systems in general.'



reactors, determining how earthquakes and other forces could affect nuclear power plants around the world. In each location, there is a unique set of conditions and engineering challenges that require customised solutions.

Modelling Disasters Before They Happen

Nuclear power plants have only been generating power since the summer of 1954, so the number of nuclear facilities to have experienced significant disasters is limited. This presents a challenge for Dr Xie's team, as they have limited realworld data to use when creating their models. To develop methods to protect nuclear reactors and other facilities from natural disasters, the team uses various analytical and numerical methods in their analyses.

Dr Xie and his colleagues develop and refine analysis models and methodologies that are applied to predict exactly how vibrations will affect nuclear reactors in order to mitigate the damage caused by earthquakes and other events. Earlier computer models were either too simple for accurate

predictions or too cumbersome for effective modelling. Since the 1970s, computer modelling has been used to predict how shaking of the ground could affect human-made structures. One factor that Dr Xie's team considers is the nature of the ground on which a reactor sits. Different types of material are present at each location and the depth of bedrock and soil layers can vary greatly. When earthquakes occur, the composition of the ground will display widely varying properties under the added strain, which will vary the motions the reactor makes as its foundations move.

Another factor to consider is that motion must be considered in three dimensions. When the earth moves beneath a structure, motion occurs in three different directions: 'forward and backward', 'left and right', and 'up and down'. This can produce rotational motions in addition to translational motions, an effect that Dr Xie and his team need to account for in their analyses.

Dr Xie and his colleagues spend a great deal of effort creating models and

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analysis methodologies that come closer to reflecting actual conditions during an earthquake. 4,14444

The objective of Dr Xie's research is to establish and improve a modern analysis framework for seismic risk analysis of nuclear power plants. To do this, his team studies four aspects of seismic risk.

For the first aspect, named 'seismic hazard analysis', the likelihood of a site to experience an earthquake of various magnitudes is determined. The second aspect is 'seismic demand analysis', where the dynamic responses of a structure experiencing earthquakes are examined.

The third aspect that the team examines is known as 'fragility analysis'. This quantifies the probability that a structure or an equipment will fail or malfunction for a certain earthquake. Through 'system analysis', the fragility of the entire nuclear power plant, which is defined as the probability that a nuclear power plant will fail to safely shutdown during an earthquake, is determined.



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Based on the results of these four analyses, Dr Xie and his colleagues are able to determine the seismic risk of a nuclear power plant in terms of core meltdown or large radioactive release.

New Models for a New World

Dr Xie and other researchers who develop methods to protect nuclear power plants from earthquakes and other catastrophes face new challenges from global climate change.

'Pavement infrastructure is experiencing unanticipated climate conditions due to global warming,' says Dr Xie. 'Extreme weather events, such as excessive precipitation, are increasing in intensity and frequency, leading to heightened concerns for pavement network vulnerability analysis, and maintenance and rehabilitation management. This is because previous designs based on historic climate may not be adequate for future conditions.' In an effort to develop infrastructure capable of withstanding increasing environmental stresses associated with global climate change, Dr Xie is collaborating with Dr Susan Tighe of the University of Waterloo. Together, the pair is developing methods to mitigate water damage to pavement infrastructure during flooding caused by extreme weather events.

Dr Xie and his team are also working closely with other organisations, including Candu Energy, a Canadian corporation that operates nuclear reactors in five countries on four continents.

Currently, there are 447 nuclear reactors generating electricity around the world, with an additional 61 currently under construction. As nuclear power plants continue to evolve and proliferate, Dr Xie and his team will continue to refine their models, creating new and improved methods to ensure safety during earthquakes, floods, and other disasters.



Meet the researcher

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Dr Wei-Chau Xie is a Professor in the Department of Civil & Environmental Engineering at the University of Waterloo in Ontario, Canada. After earning a Bachelor of Applied Science from Shanghai Jiao-Tong University in China in 1984, he received his Master's degree in Civil Engineering from the University of Waterloo in 1987, and completed his PhD in Civil Engineering there three years later. Dr Xie strives to make the world a safer place through his study on how vibrations damage structures, including nuclear power plants. He was the recipient of the Distinguished Teacher Award from the University of Waterloo in 2007 and was also awarded the Distinguished Performance Award six times, between the years of 1999 and 2013. In addition, Dr Xie was the recipient for the Doctoral Prize for Outstanding Doctoral Research from the Natural Sciences and Engineering Research Council of Canada (NSERC) in 1992. Today, Dr Xie teaches both undergraduate and graduate engineering courses, where he is beloved by his students.

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A HOLISTIC APPROACH TO THE ENERGY CRISIS

Energy surrounds us in everything that we do – it's in the sunlight that lights our world, it's in the Earth beneath our feet, and it radiates from our own bodies. Yet we are currently facing an energy crisis like no other. New technologies are needed to push past this challenge, and researchers like **Dr Saniya LeBlanc** and her team at The George Washington University are helping to get us there.



Over the past few decades, population growth and industrial development have both contributed to an increased demand for energy worldwide. As this demand continues to rise, the limited natural resources that we use to power our societies are rapidly diminishing.

In fact, we still use oil, coal and gas for the vast majority of our current energy requirements – all of which are in limited supply. We need to find ways to use energy much more efficiently to ensure that our needs can continue to be fulfilled into the future.

The energy that we use in our daily lives comes in many guises – in the form of electricity, energy powers our devices, while energy in the form of heat cooks our food and heats up our homes. We also use energy in order to drive our car to work. But in many of these processes, from charging an iPad to driving a car, energy is wasted as heat.

Indeed, laptops, PCs and tablets constantly give off wasted heat when

operating, as do much larger machines such as those involved in manufacturing chemicals, making glass and refining oil. Typically, we ignore this excess heat, or employ technology to remove it from the system that produces it. In fact, we spend billions of dollars each year on trying to cool our computers, mechanics and machinery. But what if we could use the heat instead?

This is where thermoelectric generators come in: these are devices that can turn heat directly into electricity. They work by exploiting a phenomenon known as the Seebeck effect, where heat can be directly converted into electricity using semiconductor materials. Like solar cells that convert light to electricity, thermoelectric generators have no moving parts and are based on solidstate materials. But unlike solar cells, their efficiency hasn't improved much since the early devices were invented in the 19th century. For this reason, it is still not possible to charge your iPhone using nothing more than your excess body heat.



In this era of climate change and energy shortages, a new approach is urgently needed in order to advance the technology of thermoelectric generators.

Science is not Enough

Dr Saniya LeBlanc and her team at the George Washington University devote their time to developing new energy conversion devices that could help us overcome some current limitations such as how we integrate that science with usable devices. They take a bigpicture approach as they develop new manufacturing processes, model entire energy-conversion devices (instead of just the constituent parts) and even investigate the economic factors surrounding their proposed solutions. This holistic approach has propelled Dr LeBlanc to the forefront of her field and is providing us with new weapons in the war against the energy crisis. As Dr LeBlanc explains: 'My research group develops energy technologies with novel materials and advanced manufacturing techniques. Our goal is to provide the engineering analyses and solutions to help meet the ever-increasing global energy demand.'

WWW.SCIENTIA.GLOBAI 32 'My research group develops energy technologies with novel materials and advanced manufacturing techniques. Our goal is to provide the engineering analyses and solutions to help meet the ever-increasing global energy demand.'





Advanced Manufacturing Processes

Today, a single smartphone is more powerful than all of the computing power that NASA had when they first put a man on the moon. But the fundamental science of digital computers hasn't changed: we still use transistors as electronic switches to represent 0s and 1s - and build up the entire digital world from those building blocks. What has changed in the past half-century is how those transistors are manufactured. It's due to advances in manufacturing processes that we are now able to carry around computers in our pocket that would have filled an entire building just fifty years ago.

The field of materials science is steadily supplying us with new and improved energy-conversion materials that could be used in the development of thermoelectric generators. Such materials hold the potential to claw back some of the energy lost as heat - and maybe even power your iPhone – but, so far, have been unable to realise anything as grand. 'The process of integrating materials into the devices that we will ultimately use is actually fraught with science and engineering challenges,' explains Dr LeBlanc. 'We can take a new material with unprecedented properties, put it into a device, and find a disappointing device-level performance.' She believes that part of the solution lies within the manufacturing processes.

3D printers are becoming a common utility in science and engineering labs around the world. The use of rapidprototyping techniques has enabled scientists to quickly move from concept to completion at a fraction of the previous cost of obtaining custom made parts and devices. Some extrude melted plastic from a heater nozzle, while others use a variety of chemicals that solidify on contact with each other, but all 3D printers build up their objects layer by layer in a process known as 'additive manufacturing'. What Dr LeBlanc and her team are using can be thought of as 3D printing supercharged.

They use a high-power laser to melt energy conversion materials, building up thermoelectric generators with complex structures that have never been achievable before. 'We aim to expand laser additive manufacturing to include energy conversion materials,' says Dr LeBlanc. 'We are currently investigating the link between laser processing and the resulting structure and properties of thermoelectric parts.'

This process has been used on a variety of metals and ceramics, but so far, it has never been used on semiconductor materials – a key ingredient of thermoelectric generators. In two recent papers from 2016 and 2017, Dr LeBlanc demonstrated that her team's approach would allow the fabrication of thermoelectric devices with new and complex shapes, improved integration between materials and devices, and a reduction in waste over current methods. But how do these scientists decide which materials and shapes to use?





Energy Systems Modelling and Techno-economic Analysis

In order to understand how a certain combination of materials will perform as a complete device, Dr LeBlanc employs computer models that simulate the device operation. Her team has investigated a number of materials to date and have already produced some promising results.

'Our models allow us to determine, for example, how much more electricity we could get from a device if we made certain changes to the device design. They also allow us to determine the benefit of incorporating new technologies into already existing processes,' she says. 'For instance, we can determine how much electricity could be generated from the waste heat in industrial processes or automotive exhausts.' By considering the economic factors surrounding proposed devices – such as materials, manufacturing and system costs – Dr LeBlanc is able to predict which markets a device would be most successful in and, thus, where to direct her attention.

Currently, her team is investigating the link between the laser manufacturing process and the microscopic structure of the resulting material. By experimentally measuring some key physical properties of a variety of materials, they are able to model the laser melting process for that specific material, using advanced computer modelling techniques, and hone in on the material combinations that are most promising for thermoelectric generators. Once particular combinations have been selected for further investigation, the team can test their simulated results against the real thing, as they experimentally investigate 'process-property-performance' relationships.

The road to a brighter, more energy efficient future is fraught with both science and engineering difficulties, but a new approach, developed and employed by Dr LeBlanc and her research team, promises to alleviate at least some of them. By taking a comprehensive view of entire technologies – from the manufacturing methods and component materials used, to entire system simulations, and a full economic analysis of the involved stages – they are paving the way to a world where the ever-increasing global energy demand can be met with a swathe of new technologies.

The work is far from complete, but there is no doubt that Dr LeBlanc and her team will play a pivotal role in propelling us towards an energy economy that doesn't seem so bleak.

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Meet the researcher

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Dr Saniya LeBlanc completed her Bachelor's degree in Mechanical Engineering at the Georgia Institute of Technology in 2003, before travelling to the UK to undertake an engineering Master's project at the University of Cambridge. Her second Master's degree was obtained from Stanford University in 2009, where she later completed a PhD in mechanical engineering. After working for a couple of years as a research scientist at the energy start-up Alphabet Energy, in 2014 she started her current position as assistant professor in the Department of Mechanical & Aerospace Engineering at The George Washington University. Throughout her career, Dr LeBlanc has obtained a wealth of experience in both academic and commercial environments, which has given her a unique perspective. Her holistic approach to energy-conversion devices is a prime example of her unique approach. Dr LeBlanc also uses her extensive research experience to improve engineering education, and is dedicated to training the next generation of engineers.

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SAVING THE WORLD THROUGH FERTILISER AND FUEL

At the turn of the century, two unassuming chemists collaborated on the seemingly mundane task of converting nitrogen and hydrogen into ammonia. At the end of their collaboration, they had changed the course of our civilisation forever. At the Colorado School of Mines, a new collaboration has taken place in chemical and biological engineering, between **Professor Colin Wolden** and **Professor Douglas Way.** The result is an alternative approach to creating ammonia – and it may well be just as important as its predecessor.



From left to right: Dr Simona Liguori, PhD student Zhenyu Zhang, and PhD student Tommy Fuerst

Fritz Haber and Carl Bosch might not be names that you're familiar with, but they developed a process that is widely regarded as the flame that lit the fuse to the global population explosion. Discovered by Haber and commercialised by Bosch, the Haber-Bosch Process converts nitrogen into ammonia on an industrial scale, and is now used to create an estimated 450 million tons of fertiliser every year.

Because of the benefits it had for agriculture, it is thought that the Haber-Bosch Process was the primary driving force behind the population increase, from approximately 1.6 billion people in 1900, to the estimated seven billion people we have occupying our planet today. It can be argued, quite reasonably, that no other industrial process has had a larger effect on the evolution of the human world. But was the success of the Haber-Bosch Process a double-edged sword?

The seven billion people living and breathing on Earth today are facing a crisis that surpasses any other in history. Our extensive burning of fossil fuels for energy has led to climate change, which is ravishing our planet with



abnormal temperatures and a barrage of natural disasters. Now, our supply of these fuels is due to run out any day, while our governments are failing to meet renewable energy targets and our global population continues to grow, due to our mastery of medicine, economics and – with credit due to the Haber-Bosch Process – agriculture. Some people believe that the success of our civilisation might also be our downfall, unless we act to avoid the imminent energy crisis.

In recent years, there has been a flurry of activity in research related to energy, and there are countless projects aiming to either reduce our consumption, or increase our capacity. The US Department of Energy recently identified a number of areas where dramatic reductions in energy use would be beneficial. And in the chemical processing industry, ammonia production was identified as one of the top three opportunities. In fact, the Haber-Bosch Process alone accounts for approximately 2% of the total energy expenditure of the entire world, which, according to the International Energy Agency, is the equivalent of around 18 billion barrels of oil! With so much energy put into the Haber-Bosch Process, it's

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easy to see why some researchers have begun looking for alternatives.

Professors Douglas Way and Colin Wolden are collaborating on a project that could not only improve the energy efficiency of ammonia production, but also provide a means of reducing carbon dioxide emissions (the primary driver of climate change) throughout the entire industrial world. Based at the Colorado School of Mines in the US, these two innovative chemical engineers have developed an approach that could be used to replace the Haber-Bosch Process – and might just have as grand an effect on our civilisation as its predecessor.

Nitrogen Fixation and the Haber-Bosch Process

At the most basic level, a chemical reaction is a process that converts one set of chemical substances into another. The chemicals that are mixed when a reaction takes place are known as the reactants and the resultant chemicals are called the products. Lots of chemical reactions occur naturally, including nitrogen fixation – a process that takes place in the Earth's atmosphere and converts atmospheric nitrogen (N_2) into ammonia (NH_3) and other molecules.

Atmospheric nitrogen is a relatively inert gas, meaning that it does not easily react with other chemicals without the addition of external energy. In the atmosphere, this energy is provided by lightning. The enormous energy contained within a single lightning strike – which can reach temperatures of around 30,000°C – breaks the stubborn bonds of nitrogen and allows the atoms to combine with other elements and form chemical compounds. Heating nitrogen to 30,000°C in an industrial setting would be extremely difficult, but, due to the ideal gas law – which relates the temperature, volume and pressure of a gas – we can play with other variables. In point of fact, the Haber-Bosch process combines hydrogen (from natural gas) and nitrogen (from air) at roughly 600°C and at a pressure within the range of 15–25 million pascals (300–500 times the pressure that the natural process takes place at). But in order to achieve this, a catalyst is needed to help the reaction take place.

A catalyst is a chemical or substance that increases the rate of a reaction, without really being affected itself. The Haber-Bosch Process uses a variety of catalysts – but they require temperatures of around 400°C to be effective. This is a problem, because the reaction taking place within the Haber-Bosch Process will fizzle out as the volume of the reaction product increases. In other words, the reaction is not very efficient. However, this could be improved upon using a technology known as a membrane reactor.



Membrane Reactors

A membrane reactor uses a selective barrier to separate the reactants and product of a reaction in a single step. It does this by using a membrane made up of reaction-specific materials that allow the products, but not the reactants, to pass through them. Think about using a colander to drain the water from a pot of pasta – the colander is performing a similar function to the membrane in a membrane reactor. An added advantage of using a membrane reactor is that the membrane itself can contain, or be made from, a catalyst that further simplifies the process.

'In the past 30 years, membranes made of inorganic materials have been made that can operate at temperatures above those possible with standard polymer membranes,' explains Professor Way. The problem is that no one has been able to create a membrane reactor capable of producing ammonia without significant trade-offs – until now.

Much of the energy required to make ammonia is consumed making the reactant hydrogen (H_2). Most hydrogen produced today is made through a process known as 'Steam Methane Reforming' (SMR). It reacts steam (H_2O) with methane (CH₄), in the presence of a catalyst, to produce hydrogen (H_2) and, with an additional step, carbon dioxide (CO₂) too. Unfortunately, this reaction requires very high temperature (>800°C) as well as several additional purification steps to separate H_2 from the CO₂. Professors Wolden and Way have created a membrane reactor that achieves the same result in a single step.

'By making the wall of the chemical reactor permeable to the reaction product hydrogen, several advantages are created for the SMR reaction,' explains Professor Wolden. 'You make two product streams – very pure H_2 and a very concentrated

CO₂ stream. In this way, we've combined both reaction and separation in a single unit – a concept called process intensification.' In a paper published in the journal *Separation and Purification Technology* in 2017, Professors Wolden and Way describe their stable membrane reactor that can produce hydrogen, and surpasses any other that has come before it. 'The catalytic membrane reactor obtained 98% conversion, producing above 99% purity hydrogen.' Using this approach, a refinery could reduce carbon dioxide emissions and capture the carbon dioxide upstream in a hydrogen plant. When not accumulating in the Earth's atmosphere, carbon dioxide is an extremely useful chemical for many industrial processes.

Membrane reactors are not only useful for separating a product from the reactants – they can also provide a reactant to a reaction in a special way. The traditional approach has been to use materials called 'proton conducting perovskites' (PCP) as the membrane, which have an extremely complicated atomic layout, require the application of an external voltage, and do not start to become effective until above 500°C. Professors Wolden and Way found an alternative in the much simpler 'body centred cubic' (BCC) group of materials. In contrast to PCP materials, BCC membranes have very high hydrogen permeability that increases as the temperature is reduced.

In the conventional Haber-Bosch Process, molecular hydrogen (H₂) needs to be split - or 'dissociated' - into atomic hydrogen (H) in order to combine with a nitrogen atom (N) to form ammonia (NH₃). 'In our ammonia synthesis membrane reactor, we use a metallic membrane to deliver atomic hydrogen (H) to the catalyst through permeation,' says Professor Way. 'Providing hydrogen that is already dissociated means that now H₂ and N₂ are not competing for the same catalytic sites.' Molecular nitrogen (N₂) also has to undergo the same process to be converted into N. However, a fundamental limitation of the Haber-Bosch process is that N₂ and H₂ both need to use the same sites on the catalyst in order to dissociate (and are therefore in 'competition' with each other), but, using the membrane created by Professors Wolden and Way, this problem is completely eliminated. Their new membrane reactors are actually 1-2 orders of magnitude better than the PCP approach in terms of the NH₃ synthesis rate.

The new membrane technologies developed by Professors Wolden and Way hold a potential solution to some of the serious energy and climate problems we face today. Not only have they increased the effectiveness of membrane reactor production of hydrogen to a point where it could be widely adopted in the industrial world but, by simplifying the technology, they have also introduced a flexibility that could provide untold new opportunities in chemical processing such as ammonia synthesis. The implications for real, tangible problems such as reducing global carbon dioxide emissions hold the potential to change the course of our civilisation once more.





Meet the researchers

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Professor Wolden obtained his PhD in chemical engineering from the Massachusetts Institute of Technology in 1995, before briefly working as a postdoctoral research fellow at the North Carolina State University. Since 1997, he has been based at the Colorado School of Mines, where he built his career from an assistant, to an associate, and now an accomplished professor. His research interests focus on the development of nanostructured thin-films and materials with specific applications in renewable energy. He holds a number of successful patent applications related to his work.

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E: cwolden@mines.edu W: https://chemeng.mines.edu/project/colin-wolden/ Professor J. Douglas Way completed his PhD in chemical engineering at the University of Colorado in 1986. He then worked at SRI International for three years before taking an academic position at Oregon State University in 1989. In 1993, he moved to the Colorado School of Mines, as an assistant professor. In 2003, he became a full professor within the department of chemical and biological engineering, where he obtained a number of honours and awards, including several granted patent applications. In January 2017, he became Professor Emeritus and was honoured for his work by receiving an Outstanding Faculty Member award in Chemical and Biological Engineering.

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IMPROVING ELECTRODE MICROSTRUCTURAL DYNAMICS & BATTERY PERFORMANCE

Whether it be enabling renewable technologies, mobilising electric vehicles, or powering the electronic devices we carry, batteries are essential to modern life. As technology continues to advance, high-quality, long-lasting batteries are needed more than ever. **Dr Partha P. Mukherjee** and his team at Purdue University hope to gain deeper insight into the complex interactions that happen inside lithium-ion and lithium-sulphur batteries – with the ultimate goal of improving their performance and safety.

Why We Need Efficient, Safe & Long-Lasting Batteries

In a discharging battery, chemical energy is converted into electrical energy. That electrical energy can be used to power electronic devices, vehicles, or appliances, to name a few. The best part is, once a battery has discharged some, if not all, of its electrical energy, the process can be reversed, and the battery recharged.

Batteries are critical to the 'realworld' function of many technologies. Take, for example, renewable energy technologies such as solar power. Without energy storage, excess solar energy that is captured during the day would be wasted. With energy storage, that energy can be stored and used later, especially at times when direct solar energy is unavailable. The same principle applies to many technologies that use temporary, seasonal or unpredictable sources of direct energy. The development of improved battery technologies is also essential for the widespread adoption of electric vehicles.

Dr Partha P. Mukherjee of Purdue University's School of Mechanical Engineering is committed to gaining a deeper understanding of the complex interactions associated with certain energy storage systems, for example, lithium-ion (Li-ion) and lithium-sulphur (Li-S) batteries. Armed with this knowledge, he hopes to improve their performance, longevity and safety.

A Bit About Lithium-Ion and Lithium-Sulphur Batteries

Batteries consist of three main parts the anode, cathode and electrolyte. The anode and the cathode are the negative and positive electrodes, respectively. Electrodes store electrochemical energy in the form of chemical compounds. When the battery is connected to a circuit, a transfer of charge between these electrodes is initiated. This charge then flows through objects to which the battery is connected, and the associated electrical energy is converted into other useful types of energy. The electrolyte is a material medium that allows charge to flow through it, thus completing the electrical circuit internally.



There are many different types of batteries, and they primarily differ in, or are known by, the substances used for the electrodes. Dr Mukherjee and his colleagues have focused much of their attention on lithium-ion (Li-ion) and lithium-sulphur (Li-S) batteries. The anode in a conventional Li-ion battery is usually made from graphite, and the cathode is made from a transition metal oxide that can store lithium. In an Li-S battery, such as the one studied by Dr Mukherjee, the anode is made from lithium metal and the cathode is made from carbon impregnated with sulphur.

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Li-S batteries offer higher theoretical specific energy and sulphur is an inexpensive and earth-abundant active material. Improvements to Li-S battery technologies would certainly have broad implications regarding the efficiency and practicality of many electronic devices and energy systems. However, the sources of the factors limiting the Li-S electrochemical response are fundamentally unknown. Dr Mukherjee and his team have been investigating the physicochemical problems associated with the chemistry of this type of battery.

Microstructural Factors Affect Li-S Battery Performance

Dr Mukherjee and his colleagues set about investigating the reactions taking place at the cathode in an Li-S battery. They felt that the dynamics of this reaction site, or the 'electrodeelectrolyte interface', was central to battery performance. Of particular interest to Dr Mukherjee was the formation of solid lithium sulphide at this interface. Although lithium sulphide is a product of the reaction that happens at the cathode in a Li-S battery, it can 'precipitate' and form a film on the cathode surface. This film can inhibit the supply of electrons flowing from the cathode, preventing the chemical reaction from continuing and reducing the battery's performance.

In a paper published in 2017, Dr Mukherjee and his colleagues acknowledged that this precipitation is indeed a complicated process that involves lithium sulphide molecules adhering to the cathode (adsorption), detaching from it (desorption) and diffusing through it. However, they found that the overall process is profoundly affected by primary factors, such as the reactant concentration and operating temperature. By modelling the process, they gleaned that concentration and temperature affected the growth habits of the lithium sulphide film that forms on the carbon cathode surface.

Specifically, the research team found that one of the reactants adsorbs onto the cathode slowly when present at low concentrations. This slowness, in turn, inhibits the formation of lithium sulphide 'islands'. This has a positive effect, as these 'islands' limit access to the electrode-electrolyte interface, and thus the efficiency of the reaction. The research also highlighted that an appropriate operating temperature, especially in the medium-to-high temperature range, can also improve reaction efficiency by allowing for more structured lithium sulphide growth. The team then went on to home in on the specific microstructural properties at the cathode and how they affect battery performance.





Homing in on These Complex Microstructures

In another <u>paper</u> published in 2017, Dr Mukherjee and a colleague identified the specific microstructural features that limit battery performance. In that paper, they explained that these features lead to what's known as 'surface passivation'. Passivation is the state of being passive, that is, unreactive due to an alteration of the surface layer.

As they had suggested in their earlier research, one of the main factors affecting battery performance is the formation of lithium sulphide at the electrode-electrolyte interface. As mentioned, the formation of lithium sulphide is an intrinsic part of the process and cannot be avoided. Nevertheless, the team discovered that battery performance is affected by how, or in what shape, it forms. Dr Mukherjee refers to this as the 'precipitation morphology'. Another factor they examined was cathode porosity. Porosity refers to the volume of void spaces in a material. Due to the microstructures in and around the surface of the cathode, pores can become blocked as a result of precipitation.

In summary, the team found that the microstructure growth pattern varies on the basis of precipitation morphology, leading to different build-ups due to either of these mechanisms. In turn, this produces distinct battery performance trends. They also found that the porosity of the cathode has a significant impact. Clearly, electrode microstructure is an important factor to consider when developing energy storage systems. An intimate knowledge of the related interactions would, therefore, be useful in the development of more efficient, longlasting and safe Li-S batteries.

Electrode Microstructures in Lithium-Ion Batteries

In more recent research, Dr Mukherjee and his team shifted their focus to standard Li-ion batteries. In a similar manner to the precipitation of lithium sulphide in Li-S batteries, the team demonstrated that chemically inactive solid material may partially block the active sites on the electrodes, reducing battery performance.

Another challenge related to the performance of Li-ion batteries is responding to extreme conditions. However, as suggested by Dr Mukherjee and his team, the observed responses to extreme conditions are fundamentally affected by the electrode microstructure for a given choice of materials. So, as suggested by Dr Mukherjee, adding certain structural features to the surface of electrodes could be used to overcome challenges related to extreme conditions. In line with this, the team investigated various battery 'recipes' and conditions, and found that this is indeed the case.

Understanding Microstructural Dynamics the Key

Energy storage is a central part of technological advancement. It ensures that electronic devices and other machinery are portable and available when needed. Batteries are also critical for the function of renewable energy technologies such as solar power systems and renewable transport technologies such as electric cars. In the face of climate change, we will need more powerful, efficient, and safe batteries into the future.

Dr Mukherjee and his colleagues have been working to improve energy storage technology. Specifically, they hope to gain further insights into the molecular-level interactions associated with Li-S and Li-ion batteries. So far, they have focused their work on understanding the role of microstructural features. The team has clearly demonstrated that the microstructural features of a battery's electrodes have a significant effect on performance.

Specifically, in relation to Li-S batteries, they have found that the concentration of reactants, temperature and other factors affect the formation of lithium sulphide at the electrodeelectrolyte interface. They then found, more specifically, that lithium sulphide precipitation morphology and factors related to porosity can reduce the fresh cathode surface area, hindering the reaction taking place at the cathode. This, in turn, negatively affects overall battery performance. Furthermore, in more recent research, they have demonstrated that microstructural factors also affect the performance of standard Li-ion batteries.

In conclusion, as technology continues to improve and become more powerful, we will need enhanced energy storage systems. The insight that Dr Mukherjee and his colleagues have acquired will surely help to improve the longevity, performance and safety of batteries.



Meet the researcher

Dr Partha P. Mukherjee School of Mechanical Engineering Purdue University West Lafayette, IN USA

Dr Partha P. Mukherjee received his PhD in Mechanical Engineering from Pennsylvania State University in 2007. Before moving to Purdue, he was an Assistant Professor and Morris E. Foster Faculty Fellow of Mechanical Engineering at Texas A&M University (TAMU). Prior to starting his academic career at TAMU in 2012, he worked at the US Department of Energy Labs, Oak Ridge National Laboratory, and Los Alamos National Laboratory. He currently serves as an Associate Professor of Mechanical Engineering at Purdue University, where he directs the Energy & Transport Sciences Laboratory (ETSL). Dr Mukherjee's research interests include energy storage and conversion (batteries, fuel cells), mesoscale physics and stochastics and reactive transport, materials, processing, and microstructure interactions. Some of his most recent research has been focused on lithium-ion and lithium sulphur batteries. Over the course of his career, he has been awarded many honours, including the Scialog Fellow recognition, TMS Young Leaders Award, and the Emerging Investigator Distinction from the Institute of Physics.

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WOLFSPEED & INTERNATIONAL FEMTOSCIENCE: CREATING A NEW GENERATION OF CAPACITORS

Capacitors are a vital component in virtually every electronic device we use, and yet, innovations that make them more efficient have been a long time coming. **Mr John Fraley** and his colleagues at Wolfspeed, A Cree Company, and International Femtoscience are now working on a new generation of capacitors, which they believe could offer vast improvements over current technologies. They have developed a process they hope will greatly improve the energy storage capabilities of capacitors, satisfying what has become a desperate market need.



As the world of technology advances faster than ever before, researchers at Wolfspeed and International Femtoscience believe that one type of material will ensure that the capabilities of electrical components can keep up: the wide bandgap semiconductor.

Semiconductors are instrumental in electronic systems. Essentially acting as a cross between an insulator and a conductor, they are composed of materials that can be controlled to resist electrical current to varying degrees. 'Wide bandgap' semiconductors have structural properties that make them more resistant to electrical currents than regular semiconductors, allowing them to operate at extremely high voltages.

Mr Fraley and his colleagues at Wolfspeed and International Femtoscience believe that constructing wide bandgap semiconductors with the highest possible quality materials is a key enabling technology for next generation electronics in general, and power electronics especially. Their materials of choice are silicon carbide (SiC) and gallium nitride (GaN). By fabricating semiconductors from these compounds, Wolfspeed and International Femtoscience aim to improve the performance of electrical circuits in a wide array of devices. In doing so, the companies have become well acquainted with an array of techniques in fabricating materials with highly desirable electrical properties. They have now focused their attention on using their expertise to innovate one of the most ubiquitous components in electronics: the humble capacitor.

The Champion of Electronic Circuits

Capacitors can vary wildly in construction and physical form. Most capacitors contain at least two electrical conductors which are separated by an electrical insulator. The combination conductor-insulator-conductor 'sandwich' then constitutes a twoterminal device that stores potential energy in an electric field. This electric field will result in a net positive charge on one conductor and a net negative charge on the other conductor.



After the capacitor is charged in this way, the electrons in the negativelycharged plate want to move back to their natural position – creating a current in the circuit that flows in the opposite direction to the one that was originally induced. This effect is incredibly useful, as it allows energy to be stored in the capacitor until it is needed.

More sophisticated capacitors introduce a 'dielectric' material between the two



plates. Common dielectric materials include glass, ceramic, plastic film, paper, mica, and oxide materials. The electric field that exists across the plates causes the material to become 'polarised' – in effect meaning it attracts the electrons in the negatively-charged plate while pushing them away from the positively-charged plate.

Capacitors have a wide array of uses in electronic systems. Capacitors are utilised to store energy, so that they act like temporary batteries or other types of rechargeable energy storage systems. They are used widely in power and signal processing to make filters that can discriminate between different frequencies of electrical current. They can be used to represent information by the energy stored within them. For the researchers at Wolfspeed and International Femtoscience, capacitors are critical components in their wide bandgap-based power module systems. However, current capacitor technology requires a large volume to achieve the appropriate voltage ratings for some of their high-voltage power conversion systems.

Long Awaited Advances

Mr Fraley believes that the muchanticipated improvements in dielectric materials can be realised through fabricating parallel plate capacitors utilising thin layers of diamond sandwiched between layers of a titanium-tungsten alloy, and stacking them on top of each other. As the Wolfspeed and International Femtoscience researchers describe in a report, diamond has 'exceptional physical and electrical qualities', in that remarkably high voltages can be blocked by it, allowing it to store a lot of energy. Stacking thin layers of such 'metallised' diamond would allow for very high voltage and high capacitance density components that enable highly efficient SiC power electronic systems.

The first steps taken by Mr Fraley and his colleagues in designing their new generation of capacitors were to devise a method for fabricating ultra-thin layers of exceptionally high-quality diamond. They decided on the method of 'chemical vapour deposition' (CVD), a process that involves exposing a surface to vaporised particles, and these particles are then deposited onto the surface as thin films. CVD is commonly used by Wolfspeed and International Femtoscience to procure high-quality semiconductors for a variety of purposes, giving the team the knowledge they need to plan the method.

The next challenge was to figure out the best possible stacking arrangement of diamond layers – a configuration that would allow for the strongest bonding between the layers. The researchers also needed to determine the precise atomic structure of diamond that would give rise to the most useful dielectric properties of the overall capacitor. Finally, they would need to test prototypes of their capacitors – determining the limitations of the early models, which would help them to optimise the dielectric properties of their capacitors in subsequent models.

Initiating Stack-up

To procure each stack, Mr Fraley and his colleagues used silicon wafers as the foundations on which the layers of diamond would be deposited during



the CVD process. Silicon is commonly used in procuring similar ultra-thin layers of material – it is highly inert, meaning it does not readily react with the substances it comes into contact with. On the canvas of a smooth silicon surface, CVD could be used to precisely tailor the atomic structures of the thin layers of diamond, to optimise their useful properties.

The team then sent their diamond layers off to another company, Lance Goddard Associates, for metallisation. This process is known as electron-beam physical vapour deposition and involves a device known as an electron beam evaporator. True to its name, the device emits beams of high-energy electrons, which are aimed at a metal in order to vaporise it. Similar to CVD, this vapour then forms a thin film of material on a surface.

The team at Wolfspeed and International Femtoscience observed that the atomic structures of their metallised diamond layers depended strongly on the environment in which the reaction that formed them took place. These growth conditions were found to be vitally important to the quality of the diamond – both the CVD and metallisation processes needed to be precisely engineered to optimise the dielectric properties of the layers. In the team's second report, they describe how they varied the CVD reactor environment to produce different structures of diamond, and compared the quality of these different structures.

Finding the Right Annealing Profile

Once the diamond films have been deposited, the dielectric can be further improved by subjecting the components to high temperatures, through a process technically known as 'annealing'. During this period, the atomic structure of the deposited material is decided through the rate and time over which it is heated and cooled. Material engineers can have complete control over this 'annealing profile', giving them a strong influence on several material properties of the final product.

For their diamond films, Mr Fraley and his colleagues were particularly interested in optimising the 'resistivity' – a value that describes how much the films resist electrical current. Films with a higher resistivity would have more desirable dielectric properties in a capacitor. However, finding an annealing profile that would create diamond films with the highest resistivity would require a lot of testing.

To test the quality of their metallised diamond films, the team used a piece of test equipment called a curve tracer, which is typically used to measure how the voltage of a semiconductor varies as the current passing through it is varied. In this case, the researchers used a curve tracer to analyse the electrical properties of metallised diamond films that they had fabricated using different annealing profiles. Through rigorous analysis, they would find the film with the optimised atomic structure, and the annealing profile associated with it.

Introducing a New Generation of Capacitors

Having released their third report, Mr Fraley and his colleagues have now managed to test the quality of diamond films created through a variety of annealing profiles. They are now beginning to construct early capacitor prototypes by stacking the metallised films into layers, and have also started work on fabricating an insulating casing for their capacitors. The insulating material used ensures that a minimal amount of current can escape from the capacitors, even when being tested at high voltages.

Already, the construction processes used by the researchers at Wolfspeed and International Femtoscience have produced capacitors with some highly desirable properties. The team is targeting the creation of devices that can operate at 10 kilovolts with an energy density of 30 joules per cubic centimetre – ultimately meaning they can store a huge amount of electrical energy. Thanks to the strong electrical and material capabilities of diamond films, the team's capacitors already promise to offer vast improvements over the storage capabilities of current capacitors.

As electrical components become rapidly more advanced, there is an increasingly desperate need for capacitors that can safely store more electric current. Mr Fraley is confident that his team's research will give the first solutions to satisfy this need. Once the multi-layer capacitors are successfully demonstrated commercially, he hopes that their commercialisation will quickly follow, cementing the place of Wolfspeed and International Femtoscience's new generation of capacitors in the world of modern technology.

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Meet the researchers

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David V. Kerns is Principal Engineer and CEO of International FemtoScience, Inc., in Nashville, USA. Before this, he served as a Distinguished Professor at Vanderbilt University and as Electrical Engineering Department Chair and Associate Dean of Engineering. He also served in faculty positions at several other universities, including Florida State University. Kerns was a co-founder and President of InSouth Microsystems, a company that later developed the first commercial MEMS accelerometer. He was a member of the technical staff at Bell Laboratories and also co-founded several successful technology-based companies. Kerns holds 13 patents, has published numerous journal articles, and has received many awards including the National Academy of Engineering Gordon Prize and the IEEE Third Millennium Medal.

Jim Davidson

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Jim Davidson is currently Principal Engineer and President at International FemtoScience, Inc., in Nashville, USA. Before starting this position, Davidson was Professor and Director of Vanderbilt University Microelectronics Laboratory, and he is now Professor Emeritus at Vanderbilt University. Formerly, he was Manager of Advanced Process Development and Director of Product Assurance at Harris Semiconductor, Inc., and Vice President of Operations at InSouth Microsystems Corp. Over the course of his career, Davidson has led over \$100M in applied research programs for government and industry in advanced electronic materials and microelectronic microsensors with development programs in synthetic diamond and other advanced wide bandgap semiconductors.

Stephen Minden

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Stephen Minden is a member of the Advanced Research and Development team at Cree Fayetteville/Wolfspeed. He graduated from the University of Arkansas with a BS in Mechanical Engineering. Minden has nearly 5 years of experience in extreme environment electronics packaging, advanced material applications and high-voltage system design. Over the last year, he has managed a program focusing on the design and fabrication of advanced capacitor devices utilising CVD nano-diamond thin films. Minden has authored or co-authored many publications in the areas of extreme environment electronics packaging, high-voltage electronics, and advanced material implementation.





ADDRESSING SOCIETAL CHALLENGES WITH SENSING TECHNOLOGIES

Novel sensing technologies can help us address many significant societal challenges, from making healthcare more accessible to preventing environmental damage from occurring. Therefore, much research is devoted to developing innovative sensors that are portable, inexpensive, sensitive and accurate.

In this section of the edition, we meet a diverse ensemble of engineers and scientists who are leading the charge in the development of new sensing technologies, for applications ranging from preventative medicine to environmental monitoring, and from corrosion diagnostics to leak detection.

First in this section, we focus on the development of affordable, portable, sensitive and accurate medical sensor technologies. Such medical sensors can help healthcare professionals to diagnose various medical conditions faster and more easily than using hospital-based equipment. As most medical sensors are designed to be portable and inexpensive, they can be used on large numbers of patients in the comfort of their own homes. Their ease of use allows non-specialist healthcare workers to use them, or even the patients themselves. Because of these advantages, sensors can help patients to achieve earlier and more accurate diagnoses, so that treatment can be administered or lifestyle changes can be made to delay or even reverse the onset of various medical conditions. Thus, new sensing technologies clearly show great promise for alleviating human suffering, preventing early mortality and reducing national healthcare expenditure.

Our first researcher featured in this section is Dr Madhu Bhaskaran at RMIT University, who has developed an innovative new method for producing sensors that are both stretchable and transparent. The stretchable nature of Dr Bhaskaran's devices means that they can be comfortably worn on a patient's skin, while their transparency allows light to pass through and be sensed by the 'active layer' in the device. These sensors are capable of measuring the body's physiology directly, monitoring parameters such as blood pressure, heart rate and body temperature.

Also working at the forefront of wearable healthcare technologies is Linh Le, co-founder and CEO of Bonbouton. Using his extensive expertise in the field of graphene nanotechnology, Le and his team have developed a smart shoe insole that monitors foot temperature and pressure to detect early signs of ulcers in patients with diabetes. If temperature or pressure discrepancies are detected between the left and right foot – one of the early signs of a foot ulcer – the patient is immediately



notified and steps can be taken to prevent the ulcer from developing.

Next, we showcase the work of Dr Larysa Baraban and Dr Gianaurelio Cuniberti at TU Dresden, who also apply their knowledge of nanotechnology to create low-cost, lightweight medical sensors. In one research direction, the team applied their sensor technology to the detection of deadly viruses – Ebola and bird flu. As the team strives to ensure that their sensors are cheap, rapid and reliable, these devices will be ideal for deployment in developing countries for the quick diagnosis of fast-spreading diseases. In another direction, the team developed a sensor that can be used to assess the environmental damage caused by aquatic pollutants.

Continuing with the theme of environmental pollution, we next meet Dr Bill Challener and his colleagues at GE Global Research, who have developed a disruptive new technology to detect leaks in pipelines carrying natural gas. By using optical fibres in conjunction with laser spectroscopy, the team's sensor technology can achieve an increased range that is dramatically better than currently employed technologies. The team's new method, once rolled out, will enable earlier detection of gas leaks, helping to mitigate their devastating impacts on the environment and local communities.

From here, we move on to corrosion sensing. Because of the huge financial losses associated with corrosion, there is an international push to develop better ways to detect it, so that repairs can be made before costs spiral out of control. In our next article, we meet Dr Andreas Heyn and his colleagues at the Ottovon-Guericke-University in Germany, who have contributed greatly to this area, by developing a number of novel corrosion sensing techniques.

In our final article of this section, we introduce a company called 'Innovative Imaging and Research', or 'I2R', which develops remote sensing and imaging instruments for particularly challenging situations. Here, we discuss their partnership with NASA to develop high-speed High Dynamic Range (HDR) imaging technologies for testing rocket effectiveness. These technologies are allowing NASA to finetune their rockets and enhance their capabilities, towards future space missions.



STRETCHABLE SENSORS: ELECTRONICS ON THE MOVE

Stretchable electronic devices have numerous applications in many fields, such as healthcare monitoring, communications and detecting dangerous substances. **Dr Madhu Bhaskaran** and her group at the RMIT University have developed an innovative new method for producing devices that are both stretchable and transparent.



How to Create a Stretchable Electronic Device

Stretchable electronic devices are made up of an electrical circuit that may include wires and resistors, which are used to control the flow of electric current. This circuit, often made up of metal oxide materials, sits on top of a stretchable base called a substrate.

Such devices are becoming increasingly relevant in medical fields, as their flexibility means that they can be worn by people, either against the skin or on clothes. Opto-electronic sensors are one important type of stretchable electronic devices, as they can be used to monitor certain physiological parameters. Typically, these devices either detect light (usually visible light or ultraviolet) or manipulate the light that falls on them. As well as being stretchable, opto-electronic sensors also need to be transparent, so that light can pass through the substrate material and be sensed by the active layer of material (usually a metal oxide) within the device.

These sensors are capable of measuring the body's physiology directly (for example blood pressure, heart rate and body temperature), and can produce data that needs to be processed, stored and displayed – all of which may need to be carried out on the body.

Currently, many sensors designed to be worn by people, either as a skin patch or on clothing, are made using rigid materials. For example, hard plastics, copper wires and battery power supplies are often used, which are bulky and may perform poorly when subjected to the stresses and strains of everyday living.



Dr Madhu Bhaskaran and her group at the RMIT University aimed to create transparent stretchable electronic devices that could perform accurately and repeatedly. One of the significant challenges for conformal wearable sensors and other devices worn on the body is the constant stretching and straining that they would experience as someone goes about their daily life. 'With the demand for stretchable electronics, the challenge remains in the integration of functional metal oxides with polymer stretchable plastics as we see in new bank notes,' says Dr Bhaskaran.

When designing their devices, Dr Bhaskaran's team chose a material called polydimethylsiloxane (PDMS) as a substrate, which is stretchable, transparent and non-toxic. PDMS has previously been shown to be biocompatible, and has been used in contact lenses, skin and hair products, and even as a foaming agent in some foods. The team used a thin film of a metal oxide, either indium tin oxide (ITO) or zinc oxide (ZnO) or titanium dioxide (TiO2), as the functional part of the device. These metal oxide films need to be heated to over 400°C, in order to

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make them functional – however, PDMS can only be processed at temperatures below 100°C.

To address this problem, the researchers developed a novel method. 'My team has innovatively created a technological breakthrough by overcoming an engineering challenge of combining diverse materials to realise practical, wearable sensors,' says Dr Bhaskaran.

The team first deposited a layer of ITO on a thin layer of platinum on a silicon wafer, and then heated it to 400°C to make the material transparent. After this heating process, they coated the ITO with PDMS, and embedded metal oxide resistors within this stretchable PDMS base. The platinum layer does not adhere well to the silicon wafer base, which means the PDMS and metal oxide layer, together with the platinum, can be easily peeled off the base. The team then removed the platinum layer by placing the device in chamber of gas where ions actively remove the platinum, leaving only the stretchable electronic device.

Micro-Tectonics

Dr Bhaskaran and her team then went on to test their new ITO devices. They put the devices under strain by repeated stretching, measured their transparency and visualised their surfaces using a microscope with an extremely high magnification, called a scanning electron microscope. The team found that their devices were highly transparent, as they allowed 60–80% visible light to pass through.

As mentioned previously, metal oxide materials such as ITO and ZnO are typically rigid, and this has prevented them from realising their full potential in wearable devices. Amazingly, under mechanical strain (by stretching the material repeatedly), the team's devices performed well and showed only a slight change in their electrical properties.

So, how does a brittle material like ITO maintain its functionality under strain? To answer this question, the group decided to take a close look at the microscopic structure of the metal oxide surface. Using their scanning electron



microscope, they took pictures of the surface under various degrees of strain.

What they found was amazing. The images they obtained showed that the ITO surface was made up of tiny platelike structures, which were irregularly shaped and are a couple of microns (millionths of a metre) across. The group observed that these 'microplates' had overlapping edges, and under stretching or straining, these microplates could slide over one another. To describe what they saw, the team coined the term 'micro-tectonics'.



When the surface was stretched the microplates pulled apart slightly, and when the strain was removed, the microplates slid back over each other to return to their original position. Repeated straining did not cause any undue damage to the surface. The overall motion of the microplates was thought to be caused by overlapped sections of oxide sliding over each other, which returned to their relaxed position after stretching.

Dr Bhaskaran believes that the ability of these microplates to slide over each other whilst still maintaining contact ensures that the electrical conductivity of the surface does not significantly change. Only when placed under a high degree of strain do the microplates move far enough apart to cause a break in the conductivity. The implication of micro-tectonics is that they may perform well under strain, which is likely to occur when these electronic devices are placed on the body.

Detecting Dangerous Gases and Ultraviolet Radiation

After developing their innovative production technique, the group went on to think of new ways they could use their thin stretchable electronic devices. 'This technological breakthrough has proven to be a very versatile solution allowing for the realisation of various applications,' says Dr Bhaskaran. For example, they have used their technique to create devices that can detect dangerous gases and harmful ultraviolet radiation. 'Many of these uses are of particular relevance to Australia and can be envisioned in applications such as detecting dangerous gases in mines or reducing skin cancer with widespread use of UV sensors,' Dr Bhaskaran explains. She goes on to tell us that all of her team's devices are 'as thin as a nicotine patch'.

In one particular project, the team focused on sensing the toxic gases hydrogen and nitrogen dioxide, both of which are hazardous to humans and found in many industrial applications. At low concentrations, they are colourless and odourless, which makes them hard to detect. An important property of the thin film ZnO surface is that it is oxygen deficient – this means that there are 'vacant sites' in the surface where oxygen atoms are missing. These vacancies mean that the ZnO surface can easily absorb gases such as hydrogen and nitrogen dioxide. 'They are also one of the reasons the sensors work at room temperature,' says Dr Bhaskaran. 'Thich is a sort of a first for gas sensors, which usually only work at elevated temperatures.'

When they are absorbed onto the ZnO surface, these two gases cause different effects. Hydrogen is a 'reducing gas', which means that it injects electrons into the ZnO surface, making the material more conductive and decreasing its electrical resistance. On the other hand, nitrogen dioxide is an 'oxidising gas' and it removes electrons from the ZnO surface, causing the conductivity to decrease and therefore the electrical resistance to increase. This means that changes in the electric current passed through the device can be measured and used to detect these gases.

Another novel application explored by the research group is the development of materials for smart contact lenses. Instead of using ZnO or ITO, the team embed a layer of titanium dioxide (TiO2) nano-crystals into their PDMS substrate to create a material that is capable of manipulating light. High-tech contact lenses created from this material could potentially be used to filter out harmful radiation, transmit data, collect vital information or even display information to the wearer.

However, the team's new material isn't just restricted to smart contact lenses. Because of its ability to bend and manipulate light, it can be used to create flat optical devices that can replace bulky curved lenses, such as those found in cameras or telescopes. 'Optical "metasurfaces" seek to revolutionise the realisation of optical components, where with the creation of nano-patterns of specific sizes and variation, one can engineer optical behaviour on a flat surface,' explains Dr Bhaskaran.

Future Directions

Stretchable electronic devices are rapidly evolving and may be used in numerous applications in electronics, energy harvesting and healthcare. The development of new functional materials will revolutionise the field of stretchable electronics, as they can make wearable devices much lighter, and less expensive.

Dr Madhu Bhaskaran and her group have developed a novel method for producing thin, transparent and stretchable electronic devices using zinc oxide and other metal oxides. Many of the devices created using their technique outperform their rigid counterparts, opening the door for many new applications in medical and industrial devices.



Meet the researcher

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Microsystems Research Group. She was awarded her PhD in electronic materials engineering from RMIT University, Melbourne in 2009. Dr Bhaskaran has received prestigious awards, including Australian Museum Eureka Prize for Outstanding Early Career Researcher, MIT Technology Review Most Innovative Engineers in Asia Pacific and Engineers Australia's Most Innovative Engineers, and has received significant funding of over \$4,000,000 from the Australian Research Council. She has published a wide range of publications in high quality journals and book chapters and has presented her work numerous times at national and international conferences. Her research has resulted in 4 patents being filed in both Australia and the United States.

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BONBOUTON: LEADING THE CHARGE IN WEARABLE HEALTHCARE TECHNOLOGY

At Bonbouton, **Linh Le** and his colleagues are creating a groundbreaking new range of wearable healthcare technologies. These products can track vital signs such as skin temperature and muscle motion, empowering people with the knowledge and data they need to monitor and maintain their own health.

Recent advances in microelectronics have opened the door for the development of a range of new wearable healthcare technologies. From monitoring chronic conditions such as asthma, to detecting the onset of an epileptic seizures, these devices are revolutionising how patients are cared for.

Linh Le and his team of scientists at Bonbouton are developing a whole new category of wearable healthcare technologies, powered by integrated graphene sensors that can measure and track important body vitals. With their extensive experience and track record in graphene nanotechnology breakthroughs, the scientists at Bonbouton are working to develop and release a range of products to the market that undeniably have immense scope for changing the field of healthcare.

Graphene is a widely applicable nanomaterial with uses spanning from energy storage and electronics to touch screen technology and solar powered cells. Through a patented method involving the inkjet-printing of graphene, the team at Bonbouton has created ultra-thin and ultra-flexible sensing elements, including thermal, pressure, and potentially sweat analysis, that can be embedded in clothing. Bonbouton's aim is to develop unobtrusive and comfortable ways for people to look after their health on a wide scale.

Who is Bonbouton?

Founded by Linh Le, along with several other founding team members, Bonbouton's vision is to produce a range of wearable technologies that are at the forefront of a digital healthcare breakthrough. Bonbouton's mission is simple – to provide people with the knowledge they need to make wise decisions about their own healthcare.

As the CEO of the Bonbouton, Linh is passionate about developing technologies that can detect diseases early, so that early intervention can help to stop the progression of disease. 'My father passed away in 2015 because of cancer,' he says. 'When he was diagnosed, it was already too late. That's why my current project is related to the early detection and prevention of a disease.'

Linh studied and refined graphene printing technology since his days as a doctoral student – research that ultimately led to the inkjet printing method of fabricating Bonbouton's graphene thermal sensors. Together with Malcolm, who has a background in the neurobiology of thermoregulation, the two put together their idea

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to combine materials and medical applications to create healthcare technologies.

To make their products, the team embedded their sensors into ordinary apparel. When embedded, the thin and flexible graphene thermal sensors allow unobtrusive measurements of important parameters to be taken. 'Because of its extraordinary flexibility and thinness, we envision that our "comfortable-to-wear" graphene sensor arrays can be used for constant and wireless monitoring of a variety of pathophysiological developments,' says Linh. 'Because of its extraordinary flexibility and thinness, we envision that our "comfortableto-wear" graphene sensor arrays can be used for constant and wireless monitoring of a variety of pathophysiological developments'

Foot Temperature as a Signal

right foot

left foot

A Bright Future for Diabetes Management

At present, the scientists at Bonbouton are working to release their very first product to hit the market – a proprietary smart shoe insole that monitors foot temperature to detect early signs of ulcers in diabetic patients. The extreme thinness and flexibility of Bonbouton's graphene sensors allow them to be embedded into insoles that can be comfortably worn by diabetic patients.

In both type 1 and type 2 diabetes, foot ulcers are a common and often devastating complication – arising due to reduced blood flow in the feet, and a decreased healing ability. This preventable condition can be extremely painful and serious, and in some cases, amputation of the foot may be the only solution. In the US alone, approximately 70,000 diabetic individuals lose limbs every year, which costs the healthcare system an estimated 15 billion dollars.

The insoles constantly monitor foot temperature and pressure and send this information in real-time to Bonbouton's app, which stores detailed historical data that a patient, physician, or caregiver can review. If temperature or pressure discrepancies are detected between the left and right foot – one of the early signs of a foot ulcer – the patient is immediately notified and steps can be taken earlier in the treatment continuum to prevent the ulcer from developing.

The team believes that their early diagnostic tool will not only significantly reduce the need for foot amputations, but will also improve the mortality rate amongst diabetic patients. 'I am focused on changing people's lives by developing connected devices and preventing diabetic patients from foot amputation,' says Linh.

Linh and his team are currently working to get their insoles on the market as soon as possible, so that they can start to make a big difference for diabetes sufferers in the US. 'We're in the middle of pilot studies with several hospitals and we hope to get the first product on the market as soon as late 2018,' they explain. So far, Bonbouton has been widely credited for this breakthrough innovation, and has gained a spot in the Digital Health Breakthrough Network's Spring 2017 class. The company has also won the Smart Clothing category of the Wearable Technologies Innovation World Cup of 2017, was accepted into the prestigious Entrepreneurs Roundtable Accelerator, won second place in the 2018 Diabetes Innovation Challenge, was a diabetes care finalist in the Nolahi Challenge and was also a finalist at the Lyfebulb-Novo Nordisk Innovation Summit 2017.

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The Science Behind Bonbouton's Technology

Since its discovery around a decade ago, graphene has gained a reputation as a highly desirable nanomaterial. Comprising single layers of stronglybonded carbon atoms, graphene sheets possess the properties of high mechanical strength and flexibility, making it possible to create very flexible and thin sensors out of this nanomaterial. Importantly, it also exhibits high electrical and thermal conductivity.

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When developing their technology, Linh and his colleagues at Stevens Institute of Technology experimented with inkjetprinting methods using graphene ink to produce electrically conductive graphene electrodes (electrical conductors), which were then used to produce the thermal sensors in Bonbouton's prototypes.

The inkjet-printing method, invented and patented by Linh and his team, involves the use of graphene ink that is created by suspending graphene oxide flakes in pure water. The reason for involving graphene oxide in the production process, rather than directly printing graphene electrodes, is that graphene is hydrophobic. This means that when graphene is dispersed in water to produce ink for printing, it segregates and does not form a stable dispersion.

While this problem can be counteracted by adding surfactants (such as detergent), this is an undesirable solution as surfactants reduce the ability of the end-product electrodes to store electric charge. To solve this problem, Linh proposes the use of graphene oxide flakes to produce inks for printing, which can easily and stably be dispersed in water.

The result of the inkjet-printing process is the production of graphene oxide nanosheets stacked on top of each other. To transform the printed graphene oxide into graphene electrodes, Linh's patented method then involves chemical and heat treatment on the nanosheets – a process known as thermal reduction – which can be done using an infrared heat lamp set to around 200°C.

This method is highly advantageous for producing graphene nanosheets, because of its ability to precisely print electrodes very close together – in the form of stacked sheets. In addition, the technique makes use of widely commercially-available inkjet-printers, with some degree of modification.

Linh and his team not only found an easier and commercially viable way to produce flexible graphene electrodes, which

they initially envisioned could be used to produce microsupercapacitors (devices that store electrical charge) for biomedical purposes, but they also discovered that graphene behaves as a 'negative temperature coefficient' material. This means that graphene is a highly temperature-sensitive nanomaterial that experiences a rapid reduction in electrical resistance when the temperature increases. This key property was crucial for the Bonbouton scientists to realise that their very thin, flexible and transparent inkjet-printed graphene electrodes were ideal for producing wearable thermal sensors.

Indeed, graphene thermal sensors are widely credited for being very unique temperature-sensitive materials, as their flexible and thin nature makes them ideal for making intimate skin contact. Unlike other more obtrusive and slower to respond temperature-sensitive materials – which are usually ceramic, silicon or metal-based – graphene is a particularly conformal material, and graphene thermal sensors are thought to be very well-suited for providing long-term measurements of various vital signs.

Future Prospects

The scientists at Bonbouton are continually working to improve and broaden the applicability of their unique graphene thermal sensors. The team has noted the impact of several factors on the overall efficiency of the graphene electrodes, like the spacing between ink droplets, and have more recently launched further studies that delve deeper into the sensing reliability of graphene oxide materials.

Since the company's inception, the founding team at Bonbouton has aspired to create wearable technologies that could help people track their health and alert users of various oncoming conditions. Today, using graphene thermal sensors embedded in everyday clothing, Bonbouton has made remarkable strides with their innovative technologies, paving the way forward for a new era of self-reliance and independence around personal healthcare.





Meet the researcher

Linh T. Le Bonbouton New York USA

Linh Le is the founder and CEO of Bonbouton. He was awarded his BSc in chemistry at Vietnam National University, graduating in the top 1%, followed by a Master's degree in chemical engineering at Columbia University. In 2012, he achieved a graduate certificate in project management from the Stevens Institute of Technology, where he also worked as a research assistant and technology transfer associate. Since 2015, while working with graphene technology at Bonbouton, Linh has co-invented and patented seven graphene technology methods involving inkjet-printing, including a 2015 patent on wearable graphene sensors. His research has led him to be chosen as an 'Imagine If Deep Tech' Finalist for the Innovation Forum, in addition to receiving many other honours, such as an Excellence in Research Award and an Inventor of the Year Award in 2012, to name just a few. Outside of his work, Dr Le is an enthusiastic long-distance runner, and recently acquired the title of 'ultra-marathoner'.

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PIONEERING NANOTECHNOLOGY RESEARCH FOR MACROSCALE APPLICATIONS

Good things come in small packages. **Dr Larysa Baraban, Professor Gianaurelio Cuniberti** and their colleagues at TU Dresden, Germany, are leading the charge in the application of nanotechnology in fields as diverse as biotechnology, environmental protection and point-of-care diagnostics.

Demystifying Nanotechnology

Small can be powerful. This is the thinking behind the field of nanotechnology, which involves using things that we cannot observe with the naked eye. The field has grown by leaps and bounds in the last few decades due to technological advancements in both manufacturing processes and in the development of instruments to observe the nanoscale in more detail.

One of the most exciting aspects of nanotechnology includes nanosensors, which use nanotechnology to detect and quantify different chemicals and biochemicals with very high sensitivity. These devices are often very small and portable, meaning they can be used out in the field, where traditional lab equipment can't go – such as detecting environmental pollutants, or measuring glucose levels in patients with diabetes.

Nanowire Sensor Technology for Lowcost, Lightweight Diagnostics

Recently, Professor Cuniberti, Dr Baraban and their colleagues at TU Dresden have been investigating silica-based nanowires (tiny wires that are just a few nanometres in diameter) for several applications. In addition to studying their physical properties and explaining their behaviour and conductance, the team is also leveraging their understanding of these materials towards medical applications. Nanowire-based field effect transistors are transistors in which most of the current is carried along a channel whose resistance can be controlled using electric fields. These transistors can function as nano-sized sensors. In fact, they are the most widely applicable electronic nanosensors, because of their extensive detection capabilities and their ability to be miniaturised at low cost without compromising on quality.

Both Dr Baraban and Professor Cuniberti believe that such nanosensors show great potential for clinical applications in the near future. These sensors are widely applicable, as they operate by measuring the electrical and chemical changes in solutions.

Together, the team has pioneered the understanding of the basic mechanisms behind how these nanosensors work, and have managed to apply this knowledge to real-world scenarios. They also constantly innovate and design their devices to be cheaper, faster and more reliable, making them ideal for deployment in developing countries for the rapid diagnosis of fast-spreading diseases.

Detecting Deadly Pathogens

In two proof-of-principle studies, Dr Baraban, Professor Cuniberti and their colleagues demonstrated the applicability of their silica-based nanowire sensors in successfully detecting the presence of two









dangerous viruses: Ebola and Avian Influenza (bird flu).

The avian influenza virus (H1N1), which was declared as a pandemic in 2009, poses a severe health hazard to humans. To detect this deadly virus, the team assembled a lightweight, flexible electronic device containing an array of silica nanowire sensors. Their device has the potential to be easily fabricated in large-scale. When a sample containing the influenza virus is dropped onto the flexible device, the virus's specific DNA sequence binds to the probe attached to the device, allowing the user to confirm that the virus is present. The molecular events that occur when the target sequence binds to the probe lead to changes in the surface charge that can be reliably measured as changes in electrical signals.

One of the many advantages of this system is its short detection time – the whole procedure takes only 30 minutes including handling and incubation time to detect the presence of the virus. This represents a significant improvement over current techniques, such as 'viral culture', which takes at least five days. In addition, the team's detection platform minimises the risk of false positives that often occur in other fast and highly sensitive methods, such as 'polymerase chain reaction', which amplifies all DNA in the sample. To measure the presence of the Ebola virus, the team adopted a different approach – using nanowire devices in a so-called memristor mode. A memristor is an electrical component that regulates the flow of electrical current in a circuit, and 'remembers' the amount of charge that has previously flowed through it. This characteristic has made them very popular for use as biosensors; however, they have only been used with dry samples, which is not always applicable in point-of-care diagnostics, where samples are usually wet.

Professor Cuniberti, Dr Baraban and their team figured out a way to create the first biological memristor that is compatible with liquids and is composed of a large array of siliconnanowire-based electrical devices. The team chemically modified this device to specifically bind to a matrix protein named VP40, which is predominantly found on the Ebola virus.

When a sample containing the Ebola virus is dropped onto the device, this protein binds to a probe on the device's surface, which leads to a change in the electric current that is measured. This change in electric current can be used to reveal the concentration of virus present. Interestingly, the team's device outperformed both the traditional protein quantification assays (which are the current gold standard) and other biosensors that are currently available. This represents an important contribution to the field of biosensors and point-of-care diagnostics.

Microdroplet Technology

Dr Baraban and Professor Cuniberti have also recently developed nanowire sensors in combination with a technique called droplet microfluidics. Microfluidic systems process small quantities of fluids (in this case – microdroplets) in tiny channels, allowing several parallel processes to be assessed simultaneously.

The team's ultimate goal is to create nanodevices to measure the properties of microdroplets, with a view to measuring the chemical properties of a particular sample, or measuring the concentration of a certain chemical in a sample. Since microdroplets are so small, a major advantage of this technique is that very little sample is required, which is useful for analysing precious or scarce samples.

In one approach that was published recently in the journal *Nano Letters*, the team used nanowires to measure the chemical properties of microdroplet samples. One of the chemical properties measured using this droplet microfluidic sensor was pH, which reveals how acidic or basic a substance is.



By monitoring real-time changes in pH, the researchers were able to detect the presence of glucose in the microdroplets. This application could conceivably be useful to detect glucose levels in blood samples from patients with diabetes, for example.

The glucose detection was performed using an enzyme called glucose oxidase, which accelerates the conversion of any glucose present in the solution to an intermediate chemical that is then converted into gluconic acid. The presence of gluconic acid leads to a change in the pH of the solution in time, which can be measured by the nanowires. One of the major advantages of this system is that it does not rely on optical microscopy in order to perform the measurements; rather, it is based on the chemical properties of the solution alone. Such an 'optic-less' system would be very useful in miniaturised point-ofcare diagnostics, as optical microscopy has several limitations, including a lack of a wide range of sensitivity and the fact that the sample is often destroyed during analysis.

The research team then ran their measurements using the optic-less system and compared it with traditional optic-based sensors. Interestingly, the performance of both systems was similar. These results are highly encouraging for the team, who plan to assess their droplet microfluidic sensor for other applications, such as the early detection of pathogenic bacteria, and in drug screening.

Assessing Environmental Pollution

In another application for their microdroplet technology, the team also recently tested the suitability of their system for the detection of environmental pollution. One area where pollution can be particularly disastrous is in aquatic ecosystems.

Aquatic microorganisms play an important role in global ecosystems, as they participate in the food chain at multiple levels. Paramecia, single-celled microorganisms that feed on bacteria, algae and yeasts, are particularly susceptible to environmental pollutants such as silver nitrate. This chemical, which is commonly found in disinfectants, interferes with their metabolism and induces toxicity, hindering their ability to clean their surrounding environment.

To evaluate the levels of pollution in an ecosystem, Dr Baraban, Professor Cuniberti and their colleagues developed a millifluidic device (slightly larger than a microfluidic device) to isolate and monitor the health of single paramecium cells from large volumes of samples. Each droplet contains a single paramecium, which is monitored using a spectrometer (an optical measurement device) that detects changes in the cell's fluorescence. This fluorescence signal gives a direct measure of the health of the paramecium – the signal changes if the cell has died due to contact with a pollutant such as silver nitrate. This technique has several advantages over currently available microfluidics techniques, which can only process small volumes at once.

Upon further refinement of the team's technology, this system could be used to assess the real-time environmental damage of several pollutants including silver nitrate, copper oxide and zinc oxide.

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Meet the researchers

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Professor Gianaurelio Cuniberti obtained his PhD in 1997 in Physics in a joint collaboration between the University of Genoa, Italy and the University of Hamburg, Germany. He headed the Volkswagen Foundation Research Group at the University of Regensburg, Germany from 2003 until 2007. Currently, Professor Cuniberti serves as the Chair of Materials Science and Nanotechnology at the Technical University Dresden (TU Dresden) and the Max Bergmann Center of Biomaterials in Dresden, Germany. His research focuses on nanostructured materials for molecular sensor technology, as well as quantum transport phenomena. He has also made important contributions to the theory and modelling of the electronic and structural properties of bottom-up nanoscale materials.

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Dr Larysa Baraban completed her PhD in the University of Konstanz, Germany in 2008 in the Department of Physics. After a stint as a postdoctoral researcher in the University of Pierre and Marie Curie, France, she moved to TU Dresden, Germany, where she worked as a postdoctoral research fellow from 2011 until 2013. She is currently a group leader of Bionanosensorics in the same university. Dr Baraban's research revolves around the use of nanomaterial-based biosensors and systems, flexible sensors for point-of-care diagnostics, microfluidics for high throughput biochemical analysis, artificial nano- and micromachines and magnetic soft matter.

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EXPLOITING FIBRE OPTICS FOR DETECTING PIPELINE LEAKS

Some of the best ideas in science are ones that seem completely obvious – but only after someone else has thought them up. In the world of pipeline leak detection, **Dr Bill Challener** and his team at GE Global Research have dramatically extended the range of one of the most widely used methods, by bringing together technologies from across science and engineering, in a beautifully simple way.

Whether we like it or not, our world is still extremely dependent on fossil fuels. Our use of coal for energy dates back to 1000 B.C., but, when the industrial revolution began around 1740, the whole world began to shift away from small-scale biomass energy production in favour of the fossilised remains of million-year-old plants. Coal – in all its slate-grey splendour – burned bright around the world.

The following century brought with it a growing realisation that oil could also be exploited to produce useful energy. Our new-found infatuation with one of the blackest naturally occurring substances powered economies across the globe, signifying the beginning of an energy insurrection. 2016 saw the estimated global volume of oil reserves at 1,707 billion barrels. At £35 per barrel, that's approximately £60 trillion worth of revenue in waiting: oil is big business.

Natural gas, a substance that the researchers at GE Global Research are very familiar with, was routinely used throughout the 19th century – predominantly as a light source in Britain and the USA. However, in 1885, the chemist Robert William Bunsen invented a device that would simultaneously change the subject of chemistry and the way we used natural gas forever.

The Usefulness of Natural Gas

If you have ever taken a high school chemistry class then you will probably be familiar with Robert William Bunsen. If not by name then, at least, by legacy: he was the inventor of the Bunsen burner. The Bunsen burner is a fundamental part of any chemistry teacher's apparatus that produces a gas flame and is commonly used to heat chemical solutions and elements. Although Bunsen was focusing on a specific use for his burner – chemistry - it was soon realised that, by using similar technologies, we could extend the use of natural gas to a whole host of activities: from heating our homes and cooking our food, to new manufacturing processes and electricity generation.

Combined with the global increase in oil consumption, the increased range of uses for natural gas led to the creation of a vast network of pipelines capable of delivering oil and gas across countries, continents and seas. Today, natural gas generates just over 21% of the world's electricity (second only to coal and oil) and, in the US alone, relies on over two million miles of underground pipework for transportation.

Pipeline Leak Detection

With such huge quantities of gas and oil flowing through the vast network of

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The team laying sensor tubes in a trench for outdoor field testing

pipes that stretch throughout our world, the impact of a leak could be potentially devastating: for the environment, for the communities that the pipelines run through and for the companies that own them (see, for example, <u>https://</u> en.wikipedia.org/wiki/List of pipeline accidents). It's unsurprising, then, that a substantial amount of research has been dedicated to detecting when and where leaks occur. Available techniques range from acoustic pressure waves to the use of sniffer dogs – but a select few methods are used much more than others.





The pressure monitoring method is commonly used to detect leaks by continually checking the internal pressure of a pipe: if a sudden leak occurs then the pressure will drop suddenly, indicating that there is a problem. The mass balance approach uses the principle of the conservation of mass to detect leaks: if the mass of the gas exiting a pipe is less than the mass of the gas entering it, then gas must be being lost somewhere along the line. These two techniques are useful for relatively large leaks, of >1% of the volume of flowing gas.

Vapour sensing tubes, on the other hand, are employed for detecting extremely small leaks, weeks before they can become hazardous. These are gas permeable tubes that are buried alongside the pipeline. They are kept full of air, and any leaking substance will diffuse through the gas permeable layer into the tube, which can be detected when the contents of the tube are pushed out to a sensor.

Developments in science often come with a caveat: a trade-off between requirements and capabilities. And, for the common techniques mentioned above, that trade-off is with time, sensitivity, range and localisation (the ability to tell where the leak occurs along the pipeline). Both the pressure monitoring and mass balance approaches can detect leaks very quickly, over a relatively large range, but are insensitive to small leaks. The vapour sensing method, on the other hand, can detect much smaller leaks, but is limited in range and takes a long time to provide useful information. Dr Bill Challener and his team at GE Global Research have found an ingenious way of extending the range and improving the speed of vapour-sensing tubes by using a simple optical technique that brings us back to Robert Bunsen.

Back to Bunsen: The Invention of Spectroscopy

If you were really lucky in high school, you got to see Bunsen's invention in action by burning different elements – such as sodium (Na) or phosphorous (P) – and watching the flame of the Bunsen burner change colours. This simple experiment is one that Bunsen carried out himself in the late 1800s, to characterise the 'emission spectrum' of different elements.

In science, a spectrum is simply a continuous range of wavelengths



Methane signal detected from two separate sensor tubes after a 1 hour soak, using an interrogator connected through 10+ km optical fiber to the sensor node

of light – think about how white light is made up of all the colours of the rainbow, which vary continuously from red to violet. When Bunsen burned sodium, he observed that the light given off was a bright yellow colour: rather than being a continuous range, the spectrum of sodium manifests as two sharp yellow lines. Bunsen also observed that, when viewing sunlight through a sodium-flame, the opposite happened: the spectrum of the Sun appeared with two dark lines in place of the bright ones. Through his experiments, Bunsen had invented a technique for characterising materials based on their spectra – now known as spectroscopy.

Spectroscopy is still one of the most fundamental tools scientists have, although nowadays, they are more likely to use a laser than an open flame. The spectra of lasers are extremely narrow, and in certain cases tuneable, which makes them ideal for using in spectroscopy – if we know the wavelengths at which the dark absorption bands in a material's spectrum occur.

Advancing the State of the Art

The vapour sensing method is successfully used around the globe for detecting gas and oil leaks in pipelines up to 15 kilometres in length. In this method, the sensing tube is filled with clean air and left for a period of time (known as the soak period) where any leaking gas or vapour can diffuse into the pipe through the gas permeable cladding. As the sensing tube is closed to the environment, when a leak occurs and seeps into the tube, it will remain localised at the area where the leak is situated. The gas sensors are placed at the end of the tube and, when the air is pushed out (or purged), they will pick up any indication of a leak and, using simple mathematics, the location that it occurs at with an accuracy of around 50 metres for a 10-kilometre pipeline.

The team at GE Global Research realised that they could extend the range of the vapour sensing method by 10 times. In scientific circles, a technology that can improve the current methods by an order of magnitude like this is known as *disruptive* – it is expected to change the entire field in which it is deployed. The team's approach works in a similar way to the standard vapour sensing method, except that they use laser spectroscopy combined with optical fibres to perform the gas sensing. Natural gas, for instance, has a well-defined absorption spectrum, with dark bands that are found at similar wavelengths as those used for telecommunications. This means that commercially available equipment can be used instead of developing everything from scratch.

Laser spectroscopy gives the GE technique a specificity that cuts down on cost, processing time and susceptibility to errors by honing in on the specific absorption bands of interest. In fact, by changing the laser source at one end of the pipeline, or employing a tuneable laser, the system could be used to detect many different gases or vapours. This makes the technology especially appealing for commercial use as the function of the sensing tube can be changed with minimal extra cost.

Using optical fibres in conjunction with laser spectroscopy is what allows the GE team to extend the range so dramatically – laying the fibre alongside the sensing tube means that the laser source can be placed at the beginning of the pipe instead of at the location where the sensing takes place. This simplifies the entire system by confining the power source to the pipeline pumping station and using the optical fibres to carry the laser light (which they do very well) to 'sensing nodes' sections along the sensor tube. The tube is soaked and purged in the same way as the standard method and the optical information describing whether a leak has occurred is carried back along a separate optical fibre for processing. The range of the technology is now limited by how far the fibres can carry optical information before it starts to degrade.

The system uses optical fibre technology in a second manner as well. The optical 'cell', through which the laser light passes in order to detect a potential gas leak, is composed of novel 'hollow core' fibre developed for different wavelengths by teams at OFS Fitel and the University of Bath. The conventional telecom solid core fibre carries the laser light to and from the sensor node, where the light is focused into a short segment of hollow core fibre. During the purge cycle, the small overpressure in the sensing tube is sufficient to push a small fraction of the gas in the tube into the hollow core fibre, thereby enabling spectroscopic detection of any leaking methane.

The beauty of the GE approach lies in its simplicity and effectiveness, allowing much larger stretches of pipeline to be monitored at multiple points using a single remote interrogation station, thereby minimising investment and the need for electrical power and communications at each sensing node. Once rolled out, this technology may extend the power of the sensor tube approach to much longer pipelines, enabling earlier leak detection and helping to mitigate their devastating impacts on the environment and communities across the globe.

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From left to right: Jason Karp, Bill Challener and Matthias Kasten

Meet the researcher

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Dr William (Bill) Challener is a project leader at GE Global Research – the research and development division of General Electric. He completed his undergraduate degree in physics at the Massachusetts Institute of Technology before going on to obtain his PhD at the University of California, Berkeley. He has been working in the field of physics since 1983. His extensive experience encompasses industrial research and project management in the field of optics and has led to numerous awards and honours: he was presented with the Seagate Outstanding Technical Innovation Award in 2003; given the Information Storage Industry Consortium Technical Achievement Award in 2007 and became a fellow of the American Physical Society in 2013 (to name just a few). He has acted as principal investigator for a number of federally funded projects and has invented numerous methods and techniques.

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CUTTING THE COST OF CORROSION

\$2.5 Trillion USD. That's the most recent <u>estimate</u> for how much corrosion costs us globally every year. That's about the same as the Gross Domestic Product of the entire UK. It's no wonder, then, that there is an international push for better ways to detect and repair corrosion before it becomes too costly. **Dr Andreas Heyn** of the Ottovon-Guericke-University in Magdeburg, Germany has developed methods to do just that – using algae.



Just prior to 1997, a car manufacturer known for its high-quality vehicles made some extremely poor design decisions that would dent the future pride and pocket of their loyal customers. The switch to water-based paints (from the more expensive oil-based alternatives) might have made short-term financial sense, but it led to a ticking time-bomb that the automotive industry is still recovering from today: corrosion.

The main issue is that corrosion – or in this case, the electrochemical oxidation of metal – isn't visible on the body of a car until its effects have made their way through the paintwork and protective coatings to the outer layers. By that point, the underlying damage is already severe. A quick internet search reveals that this is very much an ongoing issue that has cost customers thousands of pounds in repairs. And in most cases, as the corrosion wasn't easily detectable – it was a cost that came as a nasty surprise.

Corrosion doesn't care whether it's damaging a car, the pipework delivering clean drinking water to our homes or the Golden Gate Bridge. During metallic corrosion, charged metal atoms (ions) leave the solid metal, and subsequently react with other atoms to form compounds that are more stable than the pure metal itself. This is the case when iron atoms leach out

of steel and react with oxygen atoms to form the compound iron oxide, or rust. As Dr Andreas Heyn, of the Ottovon-Guericke-University in Magdeburg, Germany, explains: 'This is due to thermodynamics, because metals are obtained with a lot of energy from stable compounds and they strive for this stable state again.'

The speed at which this reaction occurs is what ultimately determines the lifespan of many of our products and vast areas of infrastructure. Corrosion damages buildings, increasing repair and maintenance costs; it erodes the very framework of metal bridges, putting lives at risk unless continually managed; and it destroys any scientific and technical equipment that is required to work outside of the development laboratory, in the real world.

In short, corrosion is a serious problem and streamlining how we detect and repair materials affected could save billions of dollars every year. Dr Heyn and his colleagues spend their time trying to improve on the current techniques for corrosion detection – a project that Mercedes Benz and many others might be interested in.

In much the same way as a doctor takes a holistic approach to diagnosing a patient, Dr Heyn believes that corrosion should be understood as a

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characteristic of the whole system – not just as a result of the material being used. 'In a nutshell, this idea means that corrosion is not a sole material property, as one might suppose,' he says. 'Rather, in addition to the material, the environmental conditions, the surface and the construction or the technical design also play a significant role.' Dr Heyn and his colleagues have contributed greatly to the development of a number of novel corrosion sensing techniques.

Environment Medium / Electrolyte

temperature oxygen content chloride content pH value wetting / drying additives microbial activity

Material

alloy composition distribution of elements microstructure surface processing residual stresses

CORROSION

Construction

volume / size cracks corners edges material combination aeration

Chemical Sensing for Corrosion

In the field of sensing and measurement, it can be surprisingly difficult to extract useful information without causing damage to, or completely destroying, the sample being studied. Chemical sensing is particularly tricky, as it relies on one or more chemicals reacting with the material under study to produce something which is (usually) different.

In recent years, however, a surge of research has taken place in electrochemical sensing. Electrochemical sensing uses an electrolyte (commonly a liquid solution) that reacts with a property of the material under study to produce an electrical current. In the past, this might have meant submerging an object in a beaker and measuring the electrical current across a number of probes (or electrodes) also placed in the beaker.

Increasingly, however, research is moving towards the development of powerful devices and sensors, which are smaller, more mobile and provide greater benefits to the end user than their traditional, benchtop counterparts. This high mobility approach to electrochemical sensing is of particular significance for corrosion sensing as it applies to buildings and infrastructure. In these situations, it is impossible to immerse the entire sample in an electrolyte, and having the ability to 'spit test' weak points in a structure, for instance, could save money and lives.

'Electrochemical methods have an advantage here, because with them a direct access to the elementary reactions is possible,' explains Dr Heyn. 'With more powerful instrumentation and software, it's even possible today to track corrosion in real time without causing visible corrosion. This makes very fast and almost non-destructive measurements possible, in the laboratory or directly on site at the products or the infrastructure.' Such 'point-of-care' testing means that there really is no limit to where his technology can be applied. To make electrochemical measurements even simpler and more reliable, Dr Heyn and his colleagues have been developing 'gel electrolytes'. The gel they have created is based on a material called agar, which is made up of large molecules derived from the cell walls of some types of algae. Agar dissolves in water when heated, but upon cooling, the molecules organise themselves into a network structure, trapping water within the voids.

To create their gel, Dr Heyn and his colleagues dissolve agar in specific liquid electrolytes - so that the agar network that forms contains pockets of this testing electrolyte. Their resulting gel electrolyte is stable, durable and highly transparent. 'Because of these properties, unique opportunities for corrosion diagnostics arise - with this type of gel electrolyte it is easier to carry out electrochemical investigations than with liquid electrolytes, since the test electrolyte has now been enclosed in the gel and immobilised,' explains Dr Heyn. He emphasises that he is very grateful for the financial support for this project by the German Research Foundation (DFG).



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By carefully selecting which electrolyte is used at this stage, Dr Heyn can decide how the gel will react with other materials – such as the iron ions created during the steel corrosion process. This allows him to design application-specific sensors that can be applied directly to the material of interest. This 'point-ofcare' testing approach is similar to the way a doctor applies electrode-pads to the body during an ECG. The electrolyte is no longer constricted to a bench-top beaker and can easily be taken out of the lab.

The Korropad

In the first instance, Dr Heyn and his team chose an electrolyte that visibly changes when interacting with the iron ions released from stainless steel during corrosion – the gel turns blue when it encounters them. This quick and easy method for detecting localised corrosion is available as a commercial sensor called the Korropad.

Some of the key benefits of the Korropad over other corrosion sensing techniques are time, mobility and non-destructiveness. In order to demonstrate this, Dr Heyn and his team performed some benchmarking, by measuring the corrosion resistance of steel cutlery, using the tried and tested immersion method and the newly developed Korropad. The results are startling: to achieve similar results as those obtained during a six-hour immersion test, the team only had to run their test for around ten minutes – making it 36 times faster than the standard procedure.

More recently, Dr Heyn and his colleagues have been working on further developing the technology for different applications. One example is testing the protective layer that forms on top of the zinc coating on galvanised steel. As this layer forms and interacts with its environment, it changes its protective properties depending on the climate, thus changing the corrosion rate of the whole system. By selecting a different electrolyte to that used in the Korropad – one that acts like a natural wet film such as from rain or dew – Dr Heyn's team can measure the current across the pad to provide a direct measurement of the corrosion current density. To do this, they simply apply metal electrodes (gold, platinum or simple carbon) to the gel. The corrosion current density corresponds to the layer thickness loss per year, making it easy to assess the overall state of the material. Using this new sensor, the team can easily determine what kind of future lies in store for the structure.

What's Next for the Technology?

Speaking of futures, Dr Heyn has a clear idea of the obstacles he and his team have to overcome to make this technology common place. His aim is to develop a simple solution that can be used on-site by engineers to interrogate structures on a daily basis: 'A next step in my work is the development of easy-to-use and robust sensor systems for various applications that are accepted by practicing engineers and used in their daily work. An important prerequisite for this is the standardisation of test routines.'

In this sense, standardisation means that the sensors will perform consistently well and produce output that can be collected and compared around the globe. The next step might take some time to complete, but the underlying technology is robust and structurally sound.

So, the next time you pass over a rusting bridge – or through a forgotten playground – remember that those brown-orange patches you see are a direct indication of structural integrity and a sign that its days are numbered. Go on – it might be the last chance you ever have to play on that swing.


Meet the researcher

Dr Andreas Heyn

The Institute of Materials and Joining Technology Otto-von-Guericke-Universität Magdeburg Germany

Dr Andreas Heyn was awarded his PhD from the Otto-von-Guericke-Universität in Magdeburg, Germany in 2004, after which he worked as a postdoctoral researcher at the same university. In 2008, he was offered the position of Assistant Professorship and led another team at the Bundesanstalt für Materialforschung und -prüfung (BAM) in Berlin. Since 2015, he has been working again at the Institute of Materials and Joining Technology, where his team performs research in the fields of materials and corrosion science, corrosion testing and electrochemical methods. Dr Heyn is currently working on gel-based electrolytes for application in mobile corrosion diagnostics. Throughout his career he has received numerous awards, including the Heinz-Leuze-Award of Deutsche Gesellschaft für Oberflächentechnik (DGO) - an award for a published article which explains a significant, technical scientific problem in a clear and concise manner - on two occasions. Since 2017, he has been the chair of the GfKORR working group 'Corrosion investigation and monitoring'.

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I2R – AT THE FOREFRONT OF IMAGING & REMOTE SENSING

Scientists and engineers often need tailored remote sensing instruments to understand complex phenomena. 'Innovative Imaging and Research', or 'I2R', located at the NASA John C. Stennis Space Center in Mississippi, is developing such instruments for particularly challenging imaging situations. They have, for example, partnered with NASA to develop high-speed High Dynamic Range (HDR) imaging technologies for testing rocket effectiveness and reliability in support of space exploration.

Leading the Charge in Remote Sensing Technology

Remote sensing infers information about objects or areas of interest from a distance, typically from an aircraft or satellite. Several companies and research institutions focus on developing remote sensing instrumentation for a range of applications. One such company is Innovative Imaging and Research, or I2R. Founded in 2007, I2R is a scientific based imaging company that uses observable and sensor physics, sensor calibration, custom algorithms and real-time processing to enhance the quality and versatility of remote sensing imagery. I2R is located at the NASA John C. Stennis Space Center, Mississippi, USA, alongside numerous US Federal government agencies, technology and aerospace companies and universities. I2R provides remote sensing solutions at all levels of data collection and analysis, from instrument development and calibration to post-processing algorithms and software.

I2R's founders, Mary Pagnutti (President) and Robert E. Ryan (Chief Technical Officer), each have over 30 years of engineering, imaging and sensor technology experience. In addition, I2R employs a team of highly qualified staff members, with over half the employees holding advanced degrees in fields such as mechanical and electrical engineering, mathematics, computer science and physics.

I2R has a proven record of training and developing rising talent through the employment of interns during their postsecondary education, as well as early-career postsecondary graduates. I2R was one of only four teams to be awarded participation in NASA's inaugural Early Career Initiative, or ECI. The ECI seeks to encourage creativity and innovation by engaging early career NASA employees in handson, space technology development opportunities. It also aims to establish highly collaborative work environments and enable partnerships between NASA early career innovators and the greatest minds in industry, academia and government. Indeed, I2R is a unique, innovative company, backed up by both a wealth of experience and new talent.

This combination of a highly qualified permanent staff alongside a commitment to develop the talents of early-career scientists and engineers,





potentially in collaboration with related industry and academic institutions, has led I2R to make significant contributions to a range of novel and exciting remote sensing projects, especially as applied to image capture. For example, I2R has been working closely with NASA to develop specialised High Dynamic Range (HDR) imaging technologies. These technologies have been supporting NASA scientists and engineers in their quest to understand the behaviour and improve the performance of rocket engines. I2R's goal of producing high-quality data and instrumentation extends beyond the construction of new imaging systems to include developing advanced image and video processing algorithms as well as laboratory and in-field calibrations for remote sensing systems.



Single image from a high-speed rocket plume video taken with a standard video camera (top) and using I2R's high-speed HDR video technology (bottom)



Single image from a video taken with a standard camera (left) and using I2R's near-real time high-speed HDR video technology (right)

High-Speed Colour Scientific HDR Video

Exploring our solar system, especially our closest planetary neighbours, continues to be a focus area for many scientists and engineers around the globe. These endeavours require reliable and powerful rockets that must generate incredible amounts of thrust in order to launch spacecraft and satellites into space. While rocket technology has significantly improved since its inception, there is much work to be done to fine-tune rockets and enhance their capabilities. Rockets that function incorrectly can lead to mission failure and ultimately decrease the sustainability of long-term space exploration.

Scientists and engineers employ many tools to improve rocket function. For example, cameras that capture highquality, high-speed video can be used to better understand the dynamics of rocket combustion. Engineers use this information to identify and correct anomalies that could be affecting a rocket's performance. However, traditional cameras and recording devices are easily overwhelmed by the sheer amount of intense light emitted from a rocket plume. The images produced, therefore, give little detail or information about what is happening inside the fiery exhaust plume.

To meet this challenge, the team at I2R has developed specialised imaging technology known as high-speed colour scientific High Dynamic Range imaging, or sHDR[™]. sHDR can capture and rapidly process scientific grade, extreme HDR video streams at up to 500 frames per second for limited size images. sHDR improves the ability to measure the darkest and lightest features in an image without saturation. This technology has particularly relevant application to the study of rocket plumes, which may be several orders of magnitude brighter than nearby structures. I2R has demonstrated non-saturated imaging across scenes that vary by 120 dB or six orders of magnitude in brightness.

I2R's scientific or 'sHDR' video is radiometrically and geometrically calibrated, enabling accurate measurements of brightness

temperature, position and particle velocity. Because it is geometrically calibrated, it's also computer vision ready and capable of generating accurate three-dimensional HDR video streams. sHDR can also distinguish between the subtle tone differences in a rocket's flame, producing detailed and accurate maps of the patterns and changes within the plume. The detail provided by sHDR enables scientists to find anomalies, and thus, potential inefficiencies and instabilities in the combustion process, which leads to the development of more efficient and reliable rockets.

Other current high-definition, highspeed video sensors can image across approximately three orders of magnitude and are, by comparison, low dynamic range (LDR). These current and emerging LDR technologies have difficulty simultaneously imaging an engine test article, rocket plume, and the possible hot molten debris ejected from the combustion chamber without saturation. Standard HDR methods are also nowhere near sufficient for this application. More advanced highspeed HDR technologies are being developed for the astronomical and defence communities, but are only approaching the ability to image across approximately four orders of magnitude. While there are claims that sensors on the market can image across six orders of magnitude, this is achieved through a nonlinear, logarithmic detector response that limits the precision of any scientific measurement made. HDR techniques that interleave images acquired with multiple exposure times can achieve linear imaging across six orders of magnitude, but cannot meet the high frame rate requirements of rocket engine test and launch monitoring.

I2R sees a bright future integrating sHDR into a host of other applications including additive manufacturing, robotic welding and self-driving cars, where it is critical to simultaneously monitor relatively dim and bright features within the same image.



Calibrating Low-Light, Night-Time Imaging Sensors

While it is true that low-light imaging technology is becoming more sensitive, it can be challenging to field-calibrate nighttime imaging sensors. Night-time calibration can be difficult because 'known' natural light sources (the sun or moon) are not present, and relatively dim artificial light sources, subject to unknown variations, must be used. Calibrating against an unknown variable dim light source can result in images being inconsistent over time and not representative of real phenomena.

I2R has been developing a novel technique to calibrate low-light, night-time imaging sensors for NOAA and others. Their technique relies on an 'Accurate Active Light Source', or 'AALS'. AALS is an automated, precise, field-portable light source that produces known illumination for calibration purposes. For the US government's satellite-based Visible Infrared Imaging Radiometer Suite (VIIRS) Day Night Band (DNB) sensor calibration, 'AALS' produces 4 KW of light centred within the sensor's spectral band pass at the time the satellite passes overhead. Atmospheric measurements are taken nearly simultaneously to correct for atmospheric-induced effects. After calibration, the subsequent low-light or night-time imagery is more accurate and can be used for improved time-series analyses.

Calibrated low-light imaging technology has several different applications. For example, it can be used to monitor human activity, assess light pollution and measure night-time atmospheric properties, which are not easily achievable with current technology. Powerful low-light imaging technology means there is no such thing as the 'cover of darkness'. The technology can also be used to monitor power outages after natural disasters as well as the quality and power consumption of artificial lighting in different hard to access areas.

Laboratory Camera Calibrations

Calibrating camera and sensing equipment is vital for accurate measurements in laboratory as well as in field settings.

Whatever the application for the equipment may be, many companies and institutions recognise the importance of accuracy. In response to this need, I2R offers high-precision camera calibration services. At present, they perform camera calibrations for a variety of companies ranging from Fortune 50 companies to small start-ups and universities.

For instance, in a 2016 research project, the I2R team worked to calibrate a Raspberry Pi-based camera. A Raspberry Pi is a low-cost computer the size of a credit card. Despite being relatively small, the computer has significant processing power and provides for peripherals such as cameras, which makes it perfect for imaging applications. In a paper on this project, the team demonstrated the ability of the Raspberry pi V2.1 camera module to be radiometrically calibrated to consistently produce science-grade imagery. If the team can further validate the technology and ensure that Raspberry Pi-based cameras generate accurate and repeatable results in multiple contexts, they can be used for numerous, highly technical scientific and engineering related applications. I2R foresees that such a system could serve as a low-cost imaging option for computer vision, biophotonics, remote sensing, astronomy, and security applications, to name just a few.

More from I2R on the Horizon

We have considered just a few of I2R's interesting and diverse research and development projects. There are, of course, many others on the horizon, especially in partnership with NASA. For example, I2R is starting to develop a modular, lowcost imaging system that reliably and autonomously detects dangerous hydrogen gas leaks. Hydrogen gas leaks pose a serious safety concern as they are invisible in daylight to the human eye. Not only that, but resulting hydrogen fires are intense, and an unseen hydrogen leak within a confined space can result in an explosion. Unlike current non-imaging flame sensor technologies, I2R's imaging approach can detect small hydrogen flames at ten times the distance. I2R's technology will provide accurate information about leaks in real-time, meaning that the safety and dependability of NASA's test and launch operations will be improved, with fewer false alarms, which can be costly. The technology may also see use in the energy and hydrogen fuel sectors.

In summary, I2R is a unique and cutting-edge company that aims to provide powerful remote sensing and imaging capability to varied academic, government and industry partners. The company's dynamic combination of new talent, expertise, and industry experience ensures that they will continue to support advancements in various fields of research. Indeed, the team at I2R is at the forefront of innovation in the field of imaging and remote sensing, generating versatile, economical and accurate applications within multiple industrial contexts.



About I2R

Innovative Imaging and Research (I2R) Stennis Space Center Hancock County, MS USA

Innovative Imaging and Research (I2R) was founded by Mary Pagnutti and Robert Ryan in 2007 to provide sensor calibration technology and services to the aerial and satellite mapping industry. Leveraging NASA, NOAA and internally funded research, I2R continues to provide a large range of imaging and remote sensing products to high-tech industrial, academic and governmental customers. I2R is currently working with NASA to develop scientific High Dynamic Range (sHDR[™]) and hydrogen flame imagers for use in the field of rocket science and space exploration. I2R also offers radiometric, spatial resolution and geometric camera calibration services for large aerial mapping and small UAV cameras.

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FUNDING

National Aeronautics and Space Administration (NASA) Department of Homeland Security (DHS) The National Oceanic and Atmospheric Administration (NOAA)

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FLUID MECHANICS





MOVING ONWARDS AND UPWARDS IN FLUID MECHANICS

The exciting field of the physics of fluid behaviour fundamentally underpins numerous technologies we embrace as part of our daily lives, from vehicle design to weather forecasting, and from architecture to sports. In this section of the edition, we look at important developments in fluid mechanics across diverse fields from aviation to construction. In our consideration of the pivotal work of researchers in their respective fields, the complexity and need for multifaceted approaches in fluid mechanics readily become apparent. An overarching theme in this field is the utilisation of scientific rigour for the benefit of real-world applications.

We begin by exploring the world of aviation. In the first article of this section, we showcase the work of Dr Huu Duc Vo and Dr Njuki Mureithi from École Polytechnique de Montréal who are working on a novel technique that offers a new approach to one of the most fundamental components of aircraft design – flight control. With the aim of overcoming the limitations of current designs, this work has the potential to revolutionise both the performance and efficiency of modernday aircraft.

Placing our feet back firmly back on the ground, we explore the work of Dr John Ginger of James Cook University, Australia. Important work by Dr Ginger and his colleagues examines the effect of catastrophic winds on buildings, that is, the structural response of buildings to various wind loads. Their research to date has adopted a comprehensive range of testing procedures, including full-scale studies, and this has resulted in the improvement of existing building protocols firmly rooted in experimental science for the practical and real-life benefit of communities.

We complete this section by featuring the exciting research of Dr Gustaaf Jacobs and his team at San Diego State University. His team's research focuses on understanding the farreaching applications of the interactions between shock waves, flow dynamics and turbulence. Again, we can see the importance of validating theory and prediction through empirical work. Consistent with our aim at Scientia to promote the development of our new generation of scientists, we conclude by considering Dr Jacob's work in the mentoring and training of engineering students.

IMPROVING AIRCRAFT PERFORMANCE WITH PLASMA ACTUATORS

Aeroplanes are required to change their trajectory many times during a flight. A system of adjustable surfaces that manage lift is typically used to meet this requirement. However, **Dr Huu Duc Vo** and **Dr Njuki Mureithi** from École Polytechnique de Montréal, Canada, have been working on a totally different approach to flight control – and it may eliminate the need for adjustable surfaces, which can be inefficient, especially from an economics point of view.





Dielectric Barrier Discharge actuator concept (left) and top view of plasma generated by actuator (right)

Plasma Actuation: A New Approach to Flight Control

Flight control systems are a fundamental feature of all aircraft. These systems change the lift over individual wings and tail planes to provide the moment (or torque) for roll, pitch and yaw when controlling the aircraft. Roll refers to rotation around the longitudinal axis, caused by differential lift between the two wings, and is used for steering the aircraft. Steering is also assisted by the yaw motion, which refers to rotation around the vertical axis due to net lift generation on the vertical tail plane. The pitch moment, which comes from generating lift on the horizontal tail plane, is used to tilt the nose of the aircraft up or down to change altitude.

While the actuating mechanism has evolved from cables and pulleys to hydraulic actuators and more recently electric motors, flight control still relies on movable surfaces that alter lift by changing the flow curvature over wings and tail planes. The support and pivot mechanisms associated with these surfaces add to the weight and mechanical complexity of an airframe, thus contributing to the operating (fuel), maintenance and production costs. Moreover, the volume taken up by these surfaces reduces fuel storage space that could otherwise be used to extend aircraft range.

To overcome these limitations, new, effective and structurally robust concepts for aircraft flight control without movable surfaces are being developed. One particularly promising approach utilises a device known as a 'plasma actuator'.

Dr Huu Duc Vo and Dr Njuki Mureithi from the Department of Mechanical



Engineering at École Polytechnique de Montréal, Canada, are among the leaders in the field of plasma actuation, and are seeking to establish their approach as an alternative to traditional flight control systems. Their ultimate goal is to improve aircraft performance and efficiency, resulting in cheaper aircraft acquisition and operating costs as well as lower aircraft carbon emissions through a lighter, thus more fuel-efficient, airframe.

Benefits of Plasma Actuation

Plasma actuators are based on the formation of what is known as 'plasma' between two electrodes – one of which is exposed to the air while the other is hidden in an insulating material (dielectric). Plasma (considered a fourth state of matter) is a high energy, ionised gas made up of electrically charged particles. Plasma actuators work by ionising the part of the air around the hidden electrode and turning it into a plasma.

While air is an electrical insulator, plasma is a conductor and can also be influenced by electrical and magnetic fields. In a plasma actuator, the electrically charged particles are propelled by the electric field between the two electrodes, inducing a thin jet of air parallel to the surface that can be used to alter the flow over the wings and





Flow at wing trailing edge with Plasma Gurney flap

tail planes to control an aircraft. This actuator requires relatively low power and has no moving parts that can break. Moreover, being purely electric, the actuator has a faster response time than any mechanical actuator. As such, it is perfect for aeronautical applications.

In research of 2010, Dr Vo and Dr Mureithi outlined many of the benefits associated with plasma actuators. The pair explained in their paper that 'the replacement of these [flight control] surfaces with static flight control devices [such as plasma actuators] could potentially lead to simpler and lighter wing and tail empennage designs with increased fuel containment capacity, resulting in longer flight range while reducing fabrication and maintenance costs.'

Another aspect to consider is that current systems have gaps between the movable flight control surfaces of the aircraft that cannot be eliminated or perfectly covered, which negatively affects aircraft performance. The main type of plasma actuator, known as a 'dielectric barrier discharge actuator', on the other hand, sits flush with the aircraft's exterior surfaces. This means that the actuator does not affect air flow when not in use. Dr Vo and Dr Mureithi developed two novel plasma actuation concepts for flight control, which they called the 'Plasma Gurney Flap' and 'Wing Tip Plasma Actuation', respectively.

Plasma Gurney Flap

The lift force on a body, such as a wing, increases with the net flow curvature around it. The traditional Gurney flap is a small permanent tab located on the long, trailing edge of a wing. It increases the net flow curvature around the trailing edge of the wing, which can significantly increase lift but at the cost of additional drag.

In 2010, Dr Mureithi, Dr Vo and their graduate student Shinya Ueno presented a new, innovative concept whereby one plasma actuator is placed on the suction side (top side) and the other on the pressure side (bottom side) of the wing near its trailing edge. This set-up leads to the generation of jets in opposite directions to produce the same flow curvature as a Gurney flap. The actuators can be turned on to alter lift for flight control and off when not in use, so as not to generate additional drag. Wind tunnel experiments showed that this concept can generate the same lift increase as a traditional Gurney flap and that the effects of the two individual plasma actuators are additive.

Thus, this novel concept can be used to replace traditional flight control surfaces if the strength of the plasma actuator is high enough to cope with the background flow velocity over a real aircraft.

Wing Tip Plasma Actuation

In another 2010 research project, Dr Vo and Dr Mureithi assessed whether plasma actuators could be integrated with wing tips and used to increase lift for roll control. A tip vortex is formed at the tip of a finite wing whose position and intensity has a negative influence on the lift and the drag generated near the wing tip.

Dr Vo and Dr Mureithi proposed a concept whereby plasma actuators are placed around the wing tip to disrupt the tip vortex enough to increase the wing tip lift. Computer simulations and wind tunnel experiments show that this concept could generate enough lift change for adequate roll control of the aircraft. The team's simulations also provided insight into how placement of the actuators affects lift, and how this knowledge could be applied to realworld testing. In addition, simulations showed that this concept can be used to generate lift on a zero-net lift tail plane for yaw and pitch control.



Vorticity contours showing concentrated tip vortex without actuation (left) and diffused tip vortex due to wing tip plasma actuation (right)



In summary, the two proposed novel plasma actuation flight control concepts worked well in wind tunnel experiments and represent highly promising and improved alternatives to currently used flight control systems.

Committed to Plasma Actuator Technology

Since establishing the first research program for plasma actuation in Canada in 2006, Dr Vo and Dr Mureithi continue to be leaders in the field of plasma actuation in aeronautical applications. In fact, the work discussed here gives just a few of the applications they have been studying. The team has also been looking at new plasma actuation concepts for improving the performance and efficiency of aircraft engines and in controlling flow-induced vibrations. Since 2007, Dr Vo has proposed and investigated a novel concept whereby a plasma actuator is placed in the compressor of an aircraft gas turbine engine to suppress aerodynamic instabilities, thus allowing the engine to operate at peak efficiency without fear of engine stall. The concept was patented in 2012 and has been demonstrated on both axial and centrifugal compressors in research published in 2016.

Dr Vo and Dr Mureithi have introduced plasma actuation technology to the National Research Council Canada (NRC) Gas Turbine Laboratory, with whom they have subsequently collaborated in flow control projects involving plasma actuation in aircraft engine intake ducts, compressors, combustion chambers and turbine ducts to reduce engine noise, weight, length, mechanical complexity and NOx emission.

Dr Mureithi has also been investigating the fundamental problem of the stability and bifurcation behaviour of complex flows under controlled excitation. Flow stability control capability using plasma actuators can potentially lead, for instance, to a new approach to noise control.

Last but not least, Dr Vo has also been working on improving plasma actuator models for simulations of new flow control concepts and on experimentally characterising plasma actuator performance at high pressure and temperature for future applications in aircraft engines.

Indeed, plasma actuation-based systems offer a simpler, lighter, robust and low-cost solution to improving aircraft flight control and propulsion, and this has been clearly demonstrated in Dr Vo and Dr Mureithi's various research projects. With further tweaking, plasma actuation will undoubtedly be used in future aircraft to improve their performance, resulting in cheaper acquisition and operating costs as well as lower pollution – benefits that could ultimately be passed onto the general public and to the environment.





Meet the researchers

Dr Huu Duc Vo Department of Mechanical Engineering École Polytechnique de Montréal Montreal, Quebec Canada Dr Njuki W Mureithi Department of Mechanical Engineering École Polytechnique de Montréal Montreal, Quebec Canada

Dr Huu Duc Vo received his PhD from the Massachusetts Institute of Technology in the field of aeronautics and astronautics in 2001. After working with the Canadian aircraft engine manufacturer Pratt & Whitney Canada as a senior aerodynamicist, he took up a faculty position at École Polytechnique de Montréal where he currently serves as a professor in the Department of Mechanical Engineering. His research focuses on improving aero-engine and aircraft performance through flow control, part of which involves plasma actuators. He is a leader in the field and collaborates on many related research and development projects.

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E: huu-duc.vo@polymtl.ca W: http://www.polymtl.ca/expertises/en/vo-huu-duc Dr Njuki W Mureithi received his PhD in mechanical engineering from Canada's McGill University in 1993. After completing his PhD, he accepted a position as research engineer for Mitsubishi Heavy Industries, Japan. He then spent several years in Japan as a researcher at the University of Tokyo and an associate professor at Kobe University. He joined École Polytechnique de Montréal in 2003, where he currently serves as professor in the Department of Mechanical Engineering. His research focuses on fluid-structure dynamics in industrial and aeronautical applications. He has also developed expertise in the area of plasma actuation based flow control and fluid-structure interaction control.

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UNDERSTANDING THE EFFECTS OF SEVERE WINDSTORMS ON BUILDINGS

As natural disasters are affecting an increasing number of people worldwide, risk mitigation by design is of primary concern to engineers. One of those engineers is **Dr John Ginger,** Professor of Civil Engineering and Research Director of the Cyclone Testing Station at James Cook University, Australia. His team's research focuses on the effect of catastrophic winds on buildings – principally, the effect of internal pressure and its contribution to the overall wind loads and the resulting structural response. Their work has been pivotal in developing improved building protocols.



Understanding Wind Loadings and Building Response

Strong incoming winds exert a large pressure on the external surfaces of a building. If a door or window is compromised during a storm, the wind swiftly enters the building. Once inside, the air pushes against the internal walls, exerting a sizable force, creating what is known as 'internal pressure'.

Internal pressure is a key contributor to building damage and the resulting losses. At the very least, internal pressure can cause the envelope, such as wall cladding and roof sheeting, to be dislodged, 'opening the door', as it were, to more severe structural damage. Therefore, understanding the generation of internal pressure in buildings during storms, and the factors that contribute to its magnitude, is vital for preventing damage and mitigating risk. Specifically, such awareness would improve the initial design and construction of buildings and infrastructure.

Dr John Ginger of James Cook University, Australia, has devoted much time and energy to gaining this understanding. He and his colleagues have used a range of different testing procedures in their research, including wind tunnel model tests, computational methods and most importantly, full-scale studies. Their aim is to gain insight into wind loading and structural response during catastrophic wind events. These insights, in turn, can be of use in developing of design protocols and building standards.

As was highlighted by Dr Ginger, 'numerous post-windstorm damage investigations have shown that large internal pressure (caused by a dominant opening formed by a breach in the building envelope) is the main cause of building damage, at wind speeds less than design.' The fact that buildings are being compromised during severe weather events, at wind speed levels lower than what has been deemed to be safe, is indeed concerning. But with reliable data, a better understanding of the factors affecting internal pressure, and robust mathematical techniques to estimate internal pressure, this situation could be improved, and the associated risks mitigated.

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Factors Effecting Internal Pressure

Of particular interest to Dr Ginger is how the size and location of the dominant openings (such as a broken window, open roller door or breached wall panel), and building volume affect internal pressure. In a 2010 research project, using wind tunnel tests on a model building, Dr Ginger and his team were able to deduce clear relationships between external and internal pressure and dominant opening size and building volume. Dr Ginger suggests that buildings may at times experience internal pressures equal to, or greater than, external wind pressures during a severe windstorm. 'My research objectives are to undertake studies which provide practical outcomes that benefit the community, whilst retaining an academic interest in the project. In each project, I aim to provide a better understanding of the wind loading process and structural response.'



From left to right: Mitchell Humphries, John Ginger and Geeth Bodhinayake



There are several other factors, such as flexibility of the building envelope, approach turbulence, and flow patterns, that contribute to the magnitude of internal pressures. Background porosity is another major consideration. Background porosity refers to the leakage, or escape, of wind out of openings in the building envelope. As was highlighted in a research paper of 2013, previous work had described in detail the internal pressure response of a sealed building with a dominant opening. But buildings will, due to other openings and air leakage paths, have varying degrees of background porosity. This factor had not been taken into consideration in previous research. Dr Ginger's study found that background porosity is an important factor in determining internal pressure and should be considered. Better still, his

team demonstrated that background porosity can be factored into the mathematical relationships that had been devised to estimate total internal pressure.

In fact, by reflecting upon previous research, and by conducting their own experiments, Dr Ginger and his colleagues were able to develop detailed mathematical analysis methods to estimate the internal pressures experienced by buildings during significant wind events. These formulae incorporated the many factors that Dr Ginger's team, and others, had studied, and would be key in applying the lessons they had learnt to real-world applications.

Improving Australian Building Standards

Dr Ginger's work with his team at the Cyclone Testing Station will result in improving Australian building standards, both significant and timely. In a 2015 document, prepared for the Bush Fire and Natural Hazard's CRC, Dr Ginger and his team wrote, 'Internal pressure design in Australia is currently based on limited, simplistic analysis'. They also commented on the effect this was having on building design: 'The limited design scenarios and lack of understanding by some engineers has led to a range of internal pressures being used by structural designers, with the temptation to use lower internal pressures, leading to lower cost design'. Of course, the consequences of this could be disastrous.

The team was driven to conduct both full-scale and wind tunnel testing, and to determine the internal pressures that industrial buildings may be subjected to. They wanted to get a complete understanding of the effects of building volume, flexibility, porosity, and the size and shape of openings on internal pressures, and then compare these to the specifications in current standards. In summary, their results showed that the Australian wind loading standards can underestimate internal pressure exerted on building envelopes by up to 10%.



There were further insights gained from experimentations carried out in since 2015. It became apparent that a typical industrial building, due to its simplicity of design, is an excellent tool for studying wind loadings. In addition, tests carried out on such-like buildings would also lay a foundation for the testing of more complex, multi-levelled structures. Furthermore, the study of industrial buildings can be used to easily transition between experimental findings and implementation into codes and standards.

Working with Local Companies to Improve Building Design

Dr Ginger sought to work with local companies to improve their practices too. Specifically, he wanted to optimise the design of steel, industrial-type buildings to minimise wind induced damage. A project between the Cyclone Testing Station at James Cook University, where Dr Ginger conducts his research, and the Australian Steel Institute was initiated to provide tangible benefits to the community in terms of more resilient, optimally designed buildings. The results of this research are being applied to the relevant codes governing the construction of steel industrial buildings, for example, improving both design and construction procedures.

Improved steel industrial building design may also hold out financial benefits. Given that a reduction in internal pressure of 50% will reduce building materials and cut costs by an estimated 20% on the construction of a typical industrial building, there are significant potential savings to be made, with the savings being passed on to consumers. Interestingly, approximately 8000 sheds are sold in Australia each year in high risk, cyclone affected areas. With improved practices, Dr Ginger estimates an average saving of 7% on the wholesale costs associated with shed production. This has the potential to save over five million Australian dollars each year in cyclone affected areas alone.

Offering Expertise in Post-Disaster Assessments

In 2011, the severe tropical cyclone 'Yasi' struck far-northern Queensland in Australia, making landfall near Mission Beach, 138 kilometres south of Cairns, between midnight and 1 a.m. on Thursday, the 3rd of February. The cyclone was one of the most powerful storms to have hit Queensland in recorded history – causing widespread damage and devastation. Some estimates put the total damages resulting from the event at 800 million Australian dollars. Approximately 1000 people reported serious damage to their homes, while the net loss to agricultural production was estimated to be 300 million Australian dollars.

Dr Ginger and his team from the Cyclone Testing Station carried out post-disaster investigations after cyclone Yasi. They also conducted similar investigations following other severe Australian windstorms such as cyclones 'Vance', 'Larry' and 'Debbie'. Given that wind is one of the main agents of destruction during severe weather events, their expertise in the field of wind engineering proved to be invaluable. Dr Ginger and his team have produced several reports that have been used by regulatory authorities and government departments to develop a range of responses for improving building resistance to windstorms and protecting communities.

Clearly, Dr Ginger's work has benefited the global community in many ways. And the knowledge, insights and expertise his team has shared will only continue to do so. Their research has contributed much to understanding how to reduce the damage caused to buildings and infrastructure during times of natural disaster.

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Meet the researcher

Dr John Ginger College of Science and Engineering James Cook University Townsville, Queensland Australia

Dr John Ginger completed his PhD is 1993 at the University of Queensland with a thesis entitled 'Characteristics of Large Fluctuating Pressures in Regions of Flow Separation on Roofs'. This study of the effects of wind pressure on buildings would prove to be an important feature of his research. In fact, Dr Ginger has been involved in research, testing and consulting in the field of wind engineering for several years. He has made significant contributions to the understanding of wind loading and structural response, especially during extreme weather events. His insights have been invaluable in the development of improved building standards in Australia and across the globe. He presently serves as a Professor of Civil Engineering at James Cook University (JCU), and is the Research Director of the Cyclone Testing Station (CTS) in Townsville, Australia, which he joined in 1996.

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MODELLING SHOCK WAVES AND PARTICLE INTERACTIONS IN HIGH-SPEED FLOWS

Understanding how shock waves, flow dynamics and turbulence all interact and affect the distribution of particles has applications ranging from high-speed vehicles to explosions and even ocean sediment dynamics. **Professor Gustaaf Jacobs** at San Diego State University develops computational and self-learning models and algorithms to study the dynamics of shocked particles within highspeed flows.

Shock Waves and Flow Dynamics

Shock waves can have both natural and human-made sources. One of the most extreme examples of a natural shock wave is that generated by a supernova explosion - the final deaththroes of a massive star. This dramatic event involves enormous complexity on a range of different scales, from the cosmic scale all the way down to the microscopic. This range of scales represents one of the major obstacles in modelling complex flows. If we want to be able to predict the impact of a detonation, for example, we need to understand all the physical processes and interactions involved and be able to mathematically describe them in the model at every scale.

Professor Gustaaf Jacobs at San Diego State University strives to be at the forefront of computational modelling, including machine learning and computational method development, but also understands the essential role of verifying computations through experiments and theory validation. 'Although I primarily rely on computations to understand fundamental fluid and particle transport mechanisms and instabilities,' he explains, 'I am committed to validate and verify computations through experiments and theory in collaborative efforts.'

Modelling complex flow starts with the basic principles and mathematical theories of flow dynamics. One key aspect that needs to be fully resolved is turbulence. Studies of fluid dynamics from over a century ago recognised the complexity of a fluid moving around an obstacle and identified two zones of flow: the free flow region that remains unaffected by, and does not interact with, the obstacle; and the boundary layer on the down-flow side of the obstacle, where frictional forces between the surface of the obstacle and the fluid can significantly affect flow speed and create turbulence.

The flow separates from the surface of the object on the downstream side and thins out to mix and merge into the free flow region, forming eddies and drag. How much turbulence is created is a function of many things, including the speed of the fluid and its viscosity, as well as the shape of the object. Engineers generally look to minimise drag and reduce turbulence – creating, for example, the sleek aerofoil shape of a fast car and the dimpled surface of a golf ball.





Going with the Flow

Knowing something about the dynamics of the flow and the effects of turbulence and flow separation is one thing, but being able to visualise and study it is quite another. Wind tunnels are widely used as an experimental tool for looking at boundary layer effects and turbulence. Using smoke or fog in the tunnel can give a beautiful visual overview of the airflow dynamics, while adding oil to the surface of a model can highlight the transition between laminar and turbulent flow.

Such experimental methods provide a general overview but don't provide the high level of detail required to generate

'Through innovative modelling I aim to understand complex physics problems from a fresh point of view and make new discoveries'



accurate models. Similarly, the earliest model simulations relied on poor computing power, meaning that they were largely restricted to very simplified 2-D models with coarse resolution, limited flow dynamics and a small number of particles. The main focus of Professor Jacobs has been to improve these models, taking the detailed information from the small scale experimental and theoretical studies and finding accurate and feasible ways to model full-scale, high-speed complex particle-laden flows at high resolution.

There are two frames of reference when modelling flow: the Eulerian frame, which is focussed on a specific cross-section of flow passing a certain point over time, and the Lagrangian frame, which maps the flow path of each individual particle along its path through space and time. You can think of these in terms of where you as the observer are located: in the Eulerian frame, imagine yourself on the bank of a river watching the water flow by, while in the Lagrangian frame, think of yourself as a leaf floating along with the river and the individual path of that leaf. These Eulerian-Lagrangian models are now widely used in fluid dynamics studies. The carrier fluid is modelled on a Eulerian grid, while the individual particles are points that are traced along their path using Lagrangian-based formulae, and the two are then coupled using a method called interpolation. Interpolation is used to move between different resolutions or scales in a model – it uses advanced statistical methods to generate accurate intermediate data points so that a model can smoothly transition between them.

While increased resolution is the key to making models more accurate, improving the resolution also means increasing the computational intensity – and that can get expensive. Therefore, modellers have to find ways to make their models computationally efficient. Professor Jacobs and his team have played a key role in advancing the methods needed for this.

Their approach involves grouping particles on the Lagrangian frame into clouds, which they then model as individual points ('cloud-in-cell'). They then use generalised models and different statistical methods for processes that cannot be resolved (socalled 'closure' terms) and to interpolate between different scales and grids used in the same model.

Ever increasing computer power means that scientists can improve physical models and algorithms to run models within models: they can use highresolution models to resolve the smaller scale processes and these can then be used to fine-tune a larger-scale, coarser model simulation, while still keeping computing costs down.

Complex Particle-Laden Flows

Professor Jacobs and his team have applied this work to ever more complex flows and are focussed on working out how turbulence occurs on the very small scale, and how turbulence and shock waves interact with particles within the fluid. They are generating new and more accurate models and algorithms to describe and predict this behaviour.

'My research program has coalesced around the development of models and algorithms for the high-fidelity analysis



of (mostly) high-speed turbulent flows laden with particles in environments ranging from high-speed combustors, to explosions to stratified flow near the ocean floor,' says Professor Jacobs. 'Through innovative modelling I aim to understand complex physics problems from a fresh point of view and make new discoveries.'

Applications of this research are wide ranging, including contaminant spread due to explosions, supersonic combustion, protective shields in hypersonic aircraft and the high-speed coating of electronic and aerospace components. Many applications are of relevance to aviation and as such, Professor Jacobs has worked closely with the United States Air Force. The range of applications also highlights the range of scales that need to be considered, from millimetres to kilometres and from milliseconds to days.

Together with Dr Vorobieff from the University of New Mexico, Professor Jacobs uses a shock tube, where shocks are generated in a controlled manner by rupturing a membrane that separates a high-pressure and a low-pressure gas. These experiments generate new data to assess Professor Jacobs's models of shock waves through particle-laden fluids. This helps to improve the model's small-scale physics and the overall prediction of flow.

In collaboration with Dr Udaykumar from the University of Iowa, Professor Jacobs and his team work to further improve the multi-scale algorithms and create self-learning ones based on first principle models, which can be learned at a small scale and then applied at a larger scale. This work continues to push the boundaries in terms of creating the highest resolution models, but also with the most efficient scale up, allowing the models to remain practical in terms of the computational power required. These algorithms and models build on the group's original work on the Eulerian-Lagrangian flow models but at higher resolution and in two-fluid flow regimes. The new macroscale models are able to capture the shock wave well without losing essential information about the interactions between the shock, the particles and turbulence within the flow.

The team's models have provided insights into the importance of understanding the shape and density of the initial cloud in predicting the dispersal of the particles. Particles in the dense core of the cloud, for example, will experience less acceleration than those on the lower density outer limits. Numerical algorithms are used to describe these mesoscale flow dynamics and allow the model to deal with more particles, which is a better representation of a cloud containing particles that may all behave independently depending on their positions within the cloud.

To couple between these mesoscale processes and the macroscale, the team uses meta-models (models of models). Their coupling algorithm looks at the movement of the particles and the fluid and assesses the statistical uncertainty. The macroscale model checks in with the coupling algorithm to calculate the statistics needed to best represent the mesoscale physics, including the complex interactions between the shocks, turbulence and the particles themselves.

The team is also using these methods to look at the combustion and droplet physics in liquid-fuel combustors with chemically reactive fluids. Such flow adds another level of complexity, since the droplets can merge and separate, changing size and structure over time and thus, interacting with the other phases differently.

Training and Mentoring

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Professor Jacobs is also a passionate advocate for the mentoring and training of engineering students from highschool and above, and is the founder and director of the Center for Industrial Training and Engineering Research (CITER) within SDSU.

'I have a deep appreciation of the contributions that quality education and mentoring have had in my professional development,' he says. 'I look forward to work with STEM students from underrepresented groups who are eager to make a difference and help them advance their careers.'

The aim of CITER is to equip students with the skills to thrive in industry jobs upon graduation. The centre provides them with first-hand experience of industry-driven projects and fundamental academic research. To this end, the centre has developed strong connections with many local engineering companies with whom they support internships, seminar series and online learning.



Courtesy of www.studiocarla.com

Meet the researcher

Professor Gustaaf (Guus) Jacobs Department of Aerospace Engineering San Diego State University San Diego, CA USA

Professor Gustaaf Jacobs completed his MS in aerospace engineering at Delft University of Technology in 1998. He then went on to obtain his PhD in mechanical engineering from the University of Illinois at Chicago in 2003. After a Postdoctoral Fellowship and a Visiting Assistant Professor position at Massachusetts Institute of Technology (Mechanical Engineering) and Brown University (Applied Mathematics), Dr Jacobs moved to San Diego State University (Aerospace Engineering) in 2006. He received an Air Force Office of Scientific Research Young Investigator Award in 2009 and became an Associate Fellow of the American Institute of Aeronautics and Astronautics in 2013. In 2014, he became a professor in the Department of Aerospace Engineering at San Diego State University. His research is centred on the development of models and algorithms for the study of high resolution, high-speed, particle-laden fluids. He is also the founder and director of the Center for Industrial Training and Engineering Research (CITER), which aims to prepare students for jobs in industry upon graduation.

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MATERIALS ENGINEERING



ADVANCES IN MATERIALS ENGINEERING

This section of the edition reports on some exciting developments in the field materials engineering. Despite the apparent simplicity of the materials used to create many of the devices, machines and structures that we interact with every day, the vast majority of these have been carefully and meticulously engineered precisely for their intended use. Materials engineering is a complicated but critical field – not least because new materials open up the potential for new technologies.

Throughout history, human progress has been driven by the availability of materials to enable technological advancement. We read here of the important work by researchers in this increasingly complex field, and some of the surprising advances made toward ensuring the progression and sustainability of materials engineering for the future benefit of society.

We start this section by exploring the research of Dr Thomas Voigtmann at the German Aerospace Centre. Using theoretical physics to predict the behaviour of materials we encounter in everyday life (such as glass), Dr Voigtmann aims to establish the general principles by which their mechanical properties can be engineered to our benefit. Combining theoretical prediction with empirical observation, it becomes clear how our understanding can be improved by utilising these newly developed methods. We also consider new avenues for further research in this underexplored field.

Next, we turn to the work of the Collaborative Research Centre SFB 1083. This centre brings together a large number of researchers across various prestigious institutions in Germany, with wide-ranging and diverse fields of expertise. Their shared aim, most simply put, is to better understand the physics underlying how materials with different physical properties may be combined. In this article, we can read how their work has already driven forward our understanding of the interfaces where different miniaturised materials meet and, critically, how this will benefit the development of new and important technologies.

Next, we take a look at the work of Dr Julie Mills and her colleagues at the University of South Australia and RMIT University, who are optimising a sustainable construction material called crumbed rubber concrete. The team's novel approach takes end-of-life tyres – which all too often end up as harmful waste – and uses them to replace a proportion of the sand required in the concrete mixing process. Here, we discuss how this method not only assists in reducing the environmental impact of certain construction processes, but also how crumbed rubber concrete may have significant structural benefits over concrete in its traditional form.

We finally turn to the work of Dr Ganesh Balasubramanian and his team at Lehigh University. Demonstrating the power of thinking outside the box, we discuss how the team has taken inspiration from the science of evolution to drive forward the development and optimisation of materials specific to our needs. More recent work by the team has shown how the power of supercomputing and the so-called Cuckoo Search algorithm can vastly accelerate the design of next-generation materials, contributing greatly to the exciting promises offered by materials engineering.

NON-EQUILIBRIUM MATERIALS: BRIDGING A GAP IN UNDERSTANDING

Measuring the mechanical properties of different materials by analysing their behaviour is a familiar task to many scientists and engineers. Yet for some more unusual materials, large-scale material properties are incredibly difficult to predict using current methods. **Professor Thomas Voigtmann** at the German Aerospace Centre is now investigating how these 'soft' and 'active' materials could be better understood. His team uses theoretical physics to predict the behaviour of materials, in order to establish general principles by which mechanical properties can be precisely engineered.

In our everyday lives, we interact with a wide array of materials whose properties have been carefully engineered for our convenience. We might expect these materials to behave in ways that directly reflect how we interact with them, but this isn't always the case. For some materials, including glass, properties are strongly influenced by the production process, causing the material to reflect its own past in its behaviour.

These 'history-dependent' properties can be a nuisance, but when suitable techniques are used, they can also be exploited to produce materials with desirable mechanical properties. When engineers have control over historydependent properties, they are able to improve, fine-tune and access new functions of materials.

Such a high degree of control requires a detailed understanding of the material, and it requires engineers to influence manufacturing processes on all scales, from the molecular level to the macroscopic. 'A lot is known purely empirically, which is how these materials are being engineered, and their properties are being fine-tuned and optimised to date,' explains Professor Thomas Voigtmann of the German Aerospace Centre.

Yet on smaller scales, this knowledge begins to break down. 'A lot of the fundamental physical processes that are relevant for the behaviour of such materials under strong forces are still unclear,' he adds. 'There is a gap between fundamental statistical physics and materials science that we aim to bridge with our research.'

Flowing Soft Matter

Soft materials encompass a wide variety of the substances we interact with, including food, paint and cosmetics. As soft materials flow over time, they often display fascinating properties such as 'shear thinning', where the substance appears nearly solid at rest, but flows easily as the forces applied across them increase.

Engineers can exploit these so-called 'non-equilibrium' properties to design high-performance materials, including paint that spreads easily when applied



A Prince Rupert's drop illuminated with polarised white light, and photographed under crossed polarisers – the colours arise from stresses frozen into the material

but doesn't then drip down the wall. Professor Voigtmann believes the field of theoretical 'rheology', which studies how flowing soft materials behave on a molecular level, could improve the degree of control that engineers have over these properties. Rheology aims to predict physical laws on molecular scales, using simulations of particles to predict how materials will behave on macroscopic scales. 'A lot of the fundamental physical processes that are relevant for the behaviour of soft and active materials under strong forces are still unclear. There is a gap between fundamental statistical physics and materials science that we aim to bridge with our research.'





Calculated frozen-in stress distributions in a material in a corrugated channel

History-dependent properties represent a fascinating yet largely unexplored area of rheology. Analysing the long-lasting memory effects that depend on the preparation history of a material is an important aspect of Professor Voigtmann's research. 'We try to understand how soft materials behave when they are processed and specifically how they deform mechanically,' he says. 'This is relevant in many materials we encounter every day. These include "novel" functional materials, and "active" bio-inspired materials, that are built from entities that incorporate novel ways of converting energy into motion.'

Residual Stress in Glass

For centuries, glass makers have known that residual stresses in glass strongly depend on its production process. 'Prince Rupert's drops', which are created when molten glass is dropped directly into cold water, are a particularly famous example of how these stresses work. Resembling a tadpole, the head of the solidified drop is remarkably durable, withstanding blows from a hammer. For the tail, however, even the slightest impact will cause the entire drop to shatter. This happens because 'frozen-in' stresses, which allow the material to have high stability, are rapidly relaxed when the tail is damaged.

Professor Voigtmann and his colleagues analysed the molecular mechanisms involved as stresses freeze in after molten glass begins to stop flowing. As the liquid transforms into a solid, the stresses never quite relax to zero, even after the material has stopped flowing entirely. The amount of residual stress

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in solidified glass, and its associated mechanical properties, strongly depend on how quickly the liquid was flowing in the past.

Using both computer simulations and theoretical calculations, the team demonstrated how glass production is a clear example of a history-dependent process.

Particles That Swim by Themselves

Flowing materials aren't the only substances that display non-equilibrium properties. Another area of Professor Voigtmann's research involves 'active Brownian particles' (ABPs), or 'microswimmers', which propel themselves forward through their own internal mechanisms. Examples of natural microswimmers include bacteria that propel themselves in random directions in search of food.

ABPs are good models for many biological systems and active materials, but their non-equilibrium nature makes them difficult to analyse using statistical physics. Professor Voigtmann and his colleagues aim to understand the mechanics of large systems of ABPs.

'Having understood the basic framework for many soft materials, we now turn to active materials, both as an interesting class of new materials that can be functionalised to a large degree (or offer new applications such as targeted drug delivery), and as a contribution to understand physical principles at play in biological systems,' Professor Voigtmann comments.

Crowds of Microswimmers

Systems of active particles behave in radically different ways to regular particles in thermal equilibrium. It has been a long-standing challenge for physicists to extend concepts of statistical physics to such nonequilibrium systems. Researchers now have a fairly detailed understanding of how systems of microswimmers



behave when they are packed together less tightly. For higher densities, however, ABPs slow down to form 'glassy' states, which appear to be fluid in their structure but act like a solid in their dynamics. In one study, Professor Voigtmann and his colleague Dr Alexander Liluashvili investigated how such non-equilibrium, many-body systems could be better understood using approaches rooted in theoretical physics.

Professor Voigtmann and Dr Liluashvili used their numerical methods to solve the complex equations of motions of the suspended microswimmers, allowing them to accurately describe their dynamics. They discovered a relationship between 'caging' effects, where forces between the particles keep individual microswimmers confined, and swimming forces, which weaken the overall structure to different degrees, depending on their strength.

Material Physics in Microgravity

Reference experiments for verifying the microscopic mechanisms behind macroscopic material properties require clean experimental conditions. Since synthetic ABPs are heavier than the medium in which they swim, studies of their large-scale behaviour need to be performed under conditions of weightlessness. Therefore, Professor Voigtmann, together with a team of engineers at the German Aerospace Centre and Professor Bechinger's group at the University of Konstanz, developed a device to study the random motions of microswimmers in microgravity.

In order to simulate weightlessness, the team performed their experiment on a rocket. Their first such experiment flew in 2018 on the sounding rocket MAPHEUS-07, which provided several minutes' worth of measurement time in conditions of weightlessness. Without gravity, the microswimmers tended to aggregate much more rapidly than on the ground, where gravity tends to pull them down and acts as a confounding factor in the study of their dynamics.

'This research ties into a large programme at the Institute of Materials Physics in Space of the German Aerospace Centre, where we use various microgravity platforms to uncover the physical principles of empirical material laws in various systems like metallic melts or soft materials,' Professor Voigtmann explains.

PAC-MAN Particles

Some aspects of active particles can be understood already in terms of simple model systems. Together with his collaborator Professor Tanja Schilling, Professor Voigtmann analysed how microswimmers move around inside a porous medium. They used the analogy of the well-known video game character PAC-MAN® to describe how bacteria navigate empty spaces of a porous medium in search of food.

Compared to the 'passive' motion of regular particles, PAC-MAN in the long run moves through porous structures less effectively as he devours nutrients. This is because he often reaches dead ends, and has difficulties in escaping as he has already consumed the food that first guided him there.

Computer simulations allowed Professor Voigtmann and Professor Schilling to calculate how the motion of PAC-MAN follows a power law, with parameters that vary depending on his greediness in seeking out food. Their work could now form a theoretical basis for applications that mimic biological systems of bacteria. These include methods for decontaminating groundwater by guiding bacteria through polluted soil with nutrients and recovering oil from underground reservoirs, using a similar process.

Bridging the Gap

The research of Professor Voigtmann and his colleagues has already succeeded in bridging some of the gaps between empirical observations of the properties of soft and active materials, and theoretical predictions of their behaviour. However, the field offers an incredibly wide range of lines for research and is as yet largely unexplored.

'We have developed a new method to calculate process-dependent material properties of a large class of soft materials that is based on a microscopic theory,' Professor Voigtmann concludes. 'We now want to bring our method one step closer to engineering applications, to show that there are qualitative features of material properties that are both relevant in application and cannot be captured by more simplistic empirical models.'



Meet the researcher

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Professor Thomas Voigtmann completed his PhD at the Technical University of Munich in 2003. He then carried out post-doctoral research at the University of Edinburgh and La Sapienza University of Rome, and worked as a fellow of the Zukunftskolleg of the University of Konstanz, before taking a position at the Institute of Materials Physics in Space at the German Aerospace Centre (DLR). Since 2014, Professor Voigtmann has been a Professor of the Theory of Soft Matter both at the DLR, and the Heinrich Heine University of Dusseldorf. His research interests include non-equilibrium statistical physics, the flow and yielding behaviour of amorphous materials, the dynamics of viscous liquids, metallic alloys and soft-matter systems, and the collective dynamics of active particle systems.

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COLLABORATING TO STUDY INTERFACES IN MINIATURISED MATERIALS

Creating technologies from multiple materials with different physical properties can be hugely beneficial, but the process doesn't come without its challenges. As we fabricate new devices, an understanding of the physics occurring at the interfaces where different miniaturised materials meet is now crucial, but seriously lacking. Based at Philipps-Universität Marburg, the Collaborative Research Centre SFB 1083 is a wide collaboration of researchers at institutions across Germany, who are tackling the diverse range of problems involved with these interfaces.

Scanning Transmission Electron Microscopy (STEM)



As modern technologies rapidly improve, the materials they are made from must become more and more complex. To keep up with new advances, scientists can often create useful properties in materials by bringing two or more solids into contact with each other in intricate, innovative ways. This might sound fairly simple, but in fact, the physics involved in building materials from multiple solids quickly becomes complicated.

At the heart of the issue are the elusive properties of internal interfaces – the planar surfaces where solids come into contact with each other, hidden from outside-view. Perhaps one of the most relevant examples of internal interfaces in technology today is seen in miniaturised semiconductors.

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Because of their composition, semiconductors have the remarkable ability to switch between being conductors and insulators. If the temperature of the material changes, or a voltage is applied across it in a certain direction, its conductive properties can be easily changed. These effects have made semiconductors vital components of the modern electronic devices we use every day, including transistors and diodes in computers, radios and mobile phones.



Increasingly, hybrid miniaturised semiconductors made from multiple solids are being used to allow these electronic systems to become increasingly intricate and sophisticated, and the interfaces between these solids determine many of their useful optical and electronic properties. However, miniaturisation of these hybrid semiconductors introduces a wide range of challenges, stemming from the greatly increased influence of the interface between the different solids compared with previous materials.

Typically, when scientists probe large (non-miniaturised) hybrid materials to measure their properties, the resulting signals they observe are dominated by those originating from atoms in the interiors of solids, which comprise almost their entire volume. Comparatively, far fewer atoms are found in the edges of solids, meaning the interfaces between solids have virtually no effect on the properties of the overall material. 'MDCs



For miniaturised materials, however, these interface atoms have a far greater influence, as the ratio between interface atoms and those within the interior is far greater. In semiconductors composed of graphene and metallic monolayers, for example, every atom is in contact with an atom in another material, making an understanding of the interfaces involved fundamental to understanding the properties of the overall material. Previously, our knowledge of what is happening at interfaces at a microscopic level has not kept up with improving technologies, making it increasingly difficult to engineer more desirable miniaturised semiconductors. Now, a new research collaboration known as 'SFB 1083' aims to address this problem in detail.

To solve the wide variety of issues arising from internal interfaces, SFB 1083 has brought together groups of researchers throughout Germany in fields including chemical synthesis, semiconductor physics, structure analysis, and laser spectroscopy. Using their combined expertise, the researchers use experiments with specially prepared model systems, with internal interfaces that are precisely engineered to allow their optical and electronic properties to be intricately analysed on an atomic level. In the last few years, the collaboration has followed four important lines of research, each focusing on different issues.



Analysing the Structure of Gallium **Phosphide/Silicon Interfaces**

Although internal interfaces represent definite boundaries between solids, they don't always appear as distinctive lines. For materials connected at their interfaces, the atoms on the edge of each solid appear to intermix with each other, making the interface appear blurred and unpredictable. This apparent intermixing presents difficulties to interface models that assume abrupt boundaries between solids with little mixing.

However, in one special case analysed by SFB 1083 collaborators, intermixing between two particular solids is far easier to observe. When the SFB 1083 researchers deposited the semiconducting material gallium phosphide (GaP) onto silicon (Si), they noticed that characteristic pyramids of atoms formed across the silicon surface. translating into predictable limits to the smoothness of the interface. For scientists wishing to study the behaviour of internal interfaces, this is remarkably useful.

An important step to image the imperfections in a GaP/Si surface was taken in a 2013 study, led by Kerstin Volz at Philipps-Universität Marburg. In the study, the team analysed how the performance of semiconductors grown on silicon surfaces is affected by defects on the silicon, in turn affecting the distribution of electric charge at the interface. Using a highly sensitive imaging technique called scanning transmission electron microscopy, the researchers imaged the defects to reveal



their atomic structures for the first time. Where the GaP/Si border previously seemed intermixed, images of the interface revealed a scale small enough to show abrupt boundaries between the solids. The team discovered that the defects introduced local regions of electric charge, ultimately determining the performance of the overall semiconductor.

After this study, the researchers' attention turned to how GaP/Si semiconductors could be built and fine-tuned on atomic scales. As semiconductor volume decreases, the contribution of internal interfaces becomes increasingly important, making a detailed understanding of their molecular properties all the more crucial.

In a 2016 study, the team zoomed out from the atomic scale studied in their previous work, to reveal characteristic molecular-scale structures at the GaP/ Si interface. They discovered that what appeared to be intermixing between the solids were, in fact, distinctive pyramids on the silicon surface, which formed to minimise the mechanical stresses that arise when GaP is deposited. With knowledge of this structure, descriptions of how miniaturised semiconductors could be engineered to optimise their optical and electronic properties, taking the molecular roughness of their interfaces into full account, could be made for the first time.

One particularly useful application of the research was the improvement of a new type of laser, in which electrical



charges are transferred across internal interfaces. Lasers that operate using single-solid semiconductors are difficult to create, since they must operate at low frequencies of light – created in a process in which electrons are ejected from their atoms, changing the fundamental properties of the material.

So, a fundamentally new solid-state laser was engineered by the theoretical physicists of the SFB and afterwards built, utilising the interfaces in a stack of gallium-based semiconductors. With 'W-lasers', named for the shape of the arrangements of electron energy levels in the material, transitions between solids across internal interfaces can create high frequencies, which are not strongly diminished. Using the insights gained by the collaborators, the roughness of interfaces could be carefully designed, allowing for the controlled operation of powerful lasers at high, optical frequencies. In addition, knowledge of miniaturised semiconductor interfaces could be crucial when improving miniaturised computer technology.

Transferring Charges Across Interfaces

The process of charge transfer itself is an important area of SFB 1083's research, as negatively-charged electrons do not always cross internal interfaces directly; rather, the process often occurs through charge-transfer (CT) 'excitons'. In regular materials, excitons form when a charge is excited to a higher energy level, leaving behind a 'hole', which represents where the particle would be if it moved back into its original energy level. Each exciton consists of an excited particle and its respective hole. In CT excitons, the particle and its hole form between particles on either side of the interface, ultimately allowing the two solids to interact with each other. In theory, when excited electrons move back into their respective holes, they transfer across the interface while emitting photons of light that determine the optical and electronic properties of the overall semiconductor. However, for semiconductors made from solids of different compositions, exploiting this process becomes difficult in practice. To truly understand what is happening as electrons separate and recombine, a knowledge of CT excitons is fundamentally important.

SFB 1083 researchers have now explored these issues in detail. In their study, the groups of experimental physicists Gregor Witte, Sangam Chatterjee, Martin Koch and Wolfram Heimbrodt teamed up with the groups of theoreticians Stefan Koch and Mackillo Kira. Through their work, it became possible to manipulate CT excitons selectively for the first time, using pulses of terahertz radiation (THz) and light. The investigation allowed the team to directly measure how the formation and decay of CT excitons progress over time.

For miniaturised semiconductors used in technological applications, it is important that users can carefully control the charges that are transferred by CT excitons. In a 2015 study, the team of theoreticians outlined new techniques to selectively control which charges are transferred between two solids. To understand the control mechanisms they needed to develop, the researchers first analysed the properties of CT excitons, and the relationships between pairs of particles across internal interfaces. Their calculations allowed them to develop a sequence of THz pulses, which can induce particular charges to transfer while leaving others unaffected. The researchers conducted an experiment using a theoretical model that was more precise than any previous description, and which unexpectedly revealed a fascinating additional characteristic of interfaces. The model showed directly how quantum mechanical information can be transferred between particles without the need for charge or energy transfer. This type of information transfer had never been observed before.

In addition to the need for selective charge transfer, the compositions of the solids themselves can pose significant challenges to ensuring transfers that induce useful optical and electronic properties. In many cases, the structures of the two solids can make it difficult for CT excitons to form across interfaces, meaning the materials used to build semiconductors must be carefully selected.

In 2017, the experimentalists carried out the first detailed study into how exciton formation is affected by the various different ways in which arrangements of molecules in different solids align with each other across interfaces. For the materials they used, the researchers quantified how the strength of the emitted photons of light, created when excited charges move into their respective holes and transfer across the interface, is affected by this alignment.

The insights they have gathered could be an important step in the right direction – potentially allowing engineers to choose molecular alignments that will ensure the optical and electronic properties they require.

Charge Transport at Metal-Organic Contacts

In addition to the general problems arising from the process of charges travelling across interfaces, one specific transfer case has its own important set of issues. In modern technology, miniaturised semiconductors made from combinations of metal and carbon-based (organic) materials, are becoming increasingly important, particularly for connecting organic semiconductor devices to power supplies. Devices that currently use this technology include organic solar cells and LEDs.

Metals and organic materials are remarkably useful when used together, as their combined properties are far more diverse than simply using combinations of similar materials. However, the properties of charge transfer across the interface between the materials throw up a variety of further, more specific questions.

The charge transfer process within metals, semiconductors and organic materials is now well known, and the contact between metals and inorganic semiconductors has been subject to intense research in recent decades. Yet for metal-organic interfaces, the behaviour of electrons at the interface between both material classes has hitherto been little understood, making it more difficult to precisely engineer specific properties in miniaturised organic semiconductors. This is now one of SFB 1083's most active areas of research.

As the spokesperson of the collaboration, Professor Ulrich Höfer has played a leading role in several areas of research carried out by SFB 1083, but his interests in laser spectroscopy and ultrafast phenomena at surfaces and interfaces have made metal-organic contacts a particularly important area of his research. Currently, physicists are well aware that there are unique energetic states at the interface of metals and organic compounds, ultimately due to the preliminary work of scientists at Philipps-Universität Marburg. However, physicists have only just begun to describe these new states in detail, and it is still almost completely unknown how they might be utilised.

Carrying on from the preliminary work, SFB 1083 collaborators focussed on analysing the mechanisms in which specific energy levels of electrons form at metal-organic interfaces. The research team created model systems by depositing atom-thick films of flat lying organic molecules onto welldefined single crystals of silver.

By utilising a special kind of photoelectron spectroscopy named 'two-photon photoemission' (2PPE), the researchers investigated the properties of the so-called 'interface state', which is unique to a metal-organic interface and has no counterpart in pure organic material, metal or other types of interface. This state is spatially and energetically located between the electronic states of the metal and the organic material, so it is expected to contribute substantially to the energy and charge transfer at the boundary.

Typically, new electron energy levels will form on the surfaces of metals due to the abrupt boundaries between atoms inside the material, and on the outside. In stacked materials, the interface electrons behave in similar ways – quickly dispersing across the metal surface, and quickly decaying to lower energy levels. The researchers found that the electrons could transfer across the interface over remarkably short periods of time.

Continuing this line of research, in collaboration with theoreticians from the Donostia International Physics Centre, SFB 1083 researchers aimed to discover how the lifetime of the interface state can be determined, depending on the organic material used. The team calculated wave functions and band structures from scratch, using mathematical models that describe the energetic properties and the probability of states moving in the material. The model revealed how transfer rates of electrons across the interface can be affected by a number of mechanisms, including the properties of the binding mechanism and the temperature.

Using these insights, a new model for the fundamental properties of the interface state was introduced by developing a simple description of the energetic potentials at the interface. The model was based on graphene, the simplest organic compound – consisting of atom-thick sheets of carbon. When its properties are modified slightly, graphene can be used to simulate more complex structures. The researchers discovered that the energy levels of interface electrons strongly depend on the lengths of the bonds between carbon atoms in the very first organic layer, and atoms in the metal. By experimenting with a wide range of metallic structures and carbon-metal bond lengths, the team gained an in-depth knowledge of the previously unknown interface structure that could become ubiquitous in new metal-organic contacts.

Chemo-Selective Reactions on Surfaces

Charge transfer has posed a great range of challenges to SFB 1083's researchers, but one further issue also arises from the actual process of fabricating miniaturised semiconductors from a special class of inorganic materials, which contain both organic and metal components.

Organic molecules possess 'functional groups' – sets of atoms attached to the molecule that will readily react with other molecules. However, many inorganic materials will not readily react with these groups, making it difficult to attach the materials across an interface. On the other hand, imperfections in materials such as silicon can be too reactive, making it difficult for engineers to carefully select which molecules will attach. In careful experimentation, SFB 1083's chemists adopted strategies from chemical biology by involving a particular molecule that can selectively react with silicon surfaces.

Important insights into these more selective reactions were gained in a collaboration between the research group of the chemist Ulrich Koert and the physicists Michael Dürr (Justus-Liebig-Universität Gießen) and Ulrich Höfer and colleagues at Philipps-Universität Marburg. As the building blocks for the reactions they wished to study, the researchers used a molecule named 'cyclooctyne' – consisting of a ring of eight carbon atoms, two of which are held together by three shared pairs of electrons, forming a triple bond. When cyclooctyne is adsorbed onto silicon, this triple bond will readily break down, forming a strong covalent bond with the silicon surface leaving a so-called 'dangling bond'. This highly reactive part can then be utilised to stack subsequent molecules that would typically not bind in a well-ordered structure.

In their research, the chemists synthesised several cyclooctynebased molecules with different functional groups, which were then reacted with silicon. In every case, the team observed that the organic molecules immediately formed thin layers on the silicon surface without any need for intermediate processes – a feat that had never been achieved for organic molecules before. With this chemo-selective technique, the researchers now hope that new types of miniaturised semiconductors made from



organic and inorganic materials can be grown easily, layer by layer, without the complications previously involved.

Broad Advances in Our Knowledge of Interfaces

In recent years, the SFB 1083 collaborators have made significant strides towards understanding the diverse properties of internal interfaces between different solids. Through analysing the atomic structures of the interface between gallium phosphide and silicon, they have gained a detailed knowledge of the properties that arise when materials are deposited on silicon, and how they can be accounted for in practical devices.

They have also studied the formation and decay of charge transfer excitons between different materials in detail, revealing new insights into how these transfers can be controlled through terahertz pulses, and engineered molecular alignments.

The team's examination of the interface state, forming specifically on a variety of organic molecules on metal surfaces, has also led to new insights into the electronic structure of electronic contacts. Specifically, their work revealed how electron energy levels form on metal surfaces and decay at rates that depend on the organic material composition and binding properties. The researchers implemented cyclooctyne as an anchor between functional molecules and silicon, demonstrating how organic materials can be easily and selectively reacted to silicon surfaces.

The work of SFB 1083's scientists has already contributed significantly to our fundamental understanding of the properties of internal interfaces. Their research could soon prove invaluable to the production of diverse miniaturised semiconductors, allowing the technologies we use to continue to improve.

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About SFB 1083

Collaborative Research Centre (Sonderforschungsbereich) Philipps-Universität Marburg Germany

The Collaborative Research Centre, SFB 1083, is funded by the German Research Foundation (DFG), and was established at Philipps-Universität Marburg in 2013. SFB 1083 now hosts a collaboration of over 80 scientists, including 24 principal researchers, 15 postdoctoral researchers and more than 40 PhD students. With a combined expertise encompassing many fields across physics and chemistry, the researchers share the common goal of investigating the properties of internal interfaces between different solids, composed of both organic and inorganic materials. By experimenting with accurate model systems, the collaborators aim to achieve a detailed microscopic understanding of the chemical bonding, electronic coupling, and dynamics of energy transfer at interfaces discovering how these properties vary when different types of material are used. As of 2017, SFB 1083 also includes research groups from the Universities of Gießen and Münster and the Jülich Research Centre.

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MATERIALS ENGINEERING

CRUMBED RUBBER CONCRETE: A PROMISING MATERIAL FOR SUSTAINABLE CONSTRUCTION

Crumbed rubber concrete (CRC) is a promising new material on the construction scene. Created by replacing sand with rubber particles when mixing concrete, the material promises to significantly reduce certain environmental impacts, yet its structural properties are still relatively unexplored. Researchers at the University of South Australia and RMIT University are now assessing the properties of CRC in detail. Their insights could allow us to optimise the properties of CRC for uses in infrastructure, residential buildings and industry.

Once rubber tyres have outlived their usefulness, they have a worryingly high chance of ending up as harmful waste. Between 2013 and 2014, just 5% of tyres were recycled in Australia. Of the remainder, 32% were exported, 16% were disposed of in licenced landfills, while a concerning 47% were either entirely unaccounted for, or dumped on unlicensed sites. With little economic need for them, worn-out tyres will often simply be left to decompose over many decades, and are sometimes even burned, releasing harmful pollutants into the atmosphere.

A further, seemingly unrelated environmental issue involves extracting natural sand from the ground to create concrete. Sand is a vital component in giving concrete the necessary consistency and chemical properties, yet it is becoming increasingly depleted worldwide. As we continue to construct roads, buildings and industry at an accelerating rate, the demand for sand is forcing mining companies to cause damage to natural ecosystems, particularly in sandy habitats such as beaches and rivers. One potential solution to both of these issues could come in the form of crumbed rubber concrete (CRC). This material can be created by first grinding up end-of-life tyres into small particles with a similar consistency to sand. This 'crumbed' rubber can then replace a certain percentage of the sand used in the concrete mixing process – both giving the economic usefulness of tyre rubber a new lease of life while alleviating some of the demand for natural sand.

However, as such a new material, the structural properties of CRC still need to be tested and modelled in detail before it can be widely used in construction. Therefore, Professors Julie Mills, Yan Zhuge, Bill Skinner and Dr Xing Ma at the University of South Australia (UniSA) and Professor Rebecca Gravina at RMIT University aim to gain a sufficiently indepth understanding of the properties of CRC to enable its commercial use for the first time. They also plan to develop production methods that could improve the material's functionality.

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Differences to Traditional Concrete

Since it was first created, we have known that CRC has significantly different properties to traditional concrete. Some of these differences are positive – CRC is more resistant to tensile stress, meaning it is slightly more flexible than traditional concrete, making it able to withstand impacts more effectively. However, since there is a limited cohesion between rubber crumbs and concrete particles, CRC suffers several disadvantages in its



mechanical properties, including a generally lower compressive strength and workability than traditional concrete.

Initial studies into the potential usefulness of CRC focused on how the material could be used in footings and slabs. These structures are less dependent on concrete strength, yet account for around 40% of all concrete consumption in Australia, already showing promise for the practicality of CRC. However, the UniSA and RMIT University researchers believe the role of CRC may not need to be limited to structures that are less dependent on strength. In several recent studies, they have shown that a wide variety of techniques in the CRC production processes can be used to improve its structural properties.

In 2016, the researchers carried out a study to determine how the strength of CRC is affected by the size and shape of the rubber particles used, as well as the amount of rubber used as a percentage of the total concrete mixture. They found that simple crumbs of rubber were indeed more effective at increasing CRC strength, as opposed to other shapes such as fibres and chips. The team also concluded that the strength of CRC varies depending on the percentage of rubber used, along with the grading of the combined sizes of rubber crumbs. However, more work would be needed to quantify the optimal percentages of these values.

The team's study highlighted several further lines of investigation that would be needed to improve CRC strength. The first of these involved investigating various techniques where rubber crumbs are pre-treated with chemicals or other treatments to improve cohesion with concrete particles. Additionally, the researchers hoped to explore the dynamic responses of CRC with different percentages of rubber, investigate how the strength of reinforced concrete would be affected by the bond between CRC and steel, and develop methods to model the properties of CRC numerically.

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Treating Rubber

In a 2018 study, the UniSA and RMIT University researchers investigated how strong, workable CRC can be achieved by pre-treating rubber crumbs with a wide variety of additives. This type of research had been carried out before by other groups, but the results until then had been highly variable and often contradictory. To improve the reliability of the results, the team carried out a series of new experiments, using sophisticated imaging techniques to analyse them.

Firstly, they coated rubber crumb surfaces with chemicals including sodium chloride, sulfuric acid and potassium permanganate, and also tried soaking them in tap water as well as heating them in ovens before mixing. After treatment, the crumbs were analysed using two specialised techniques. The first of these was x-ray photoelectron spectroscopy, which allowed the researchers to accurately measure the chemical composition of the rubber crumb surfaces. Secondly, they used a scanning electron

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microscope, which enabled them to directly image the crumb surfaces to the precision of single atoms. Using these imaging techniques, the researchers could assess the effects of pretreatment on a molecular scale, providing detailed insights into how much CRC workability and strength were improved by each treatment method.

Remarkably, the team showed that pre-treating the rubber crumbs with water was more effective than any other chemical in maximising the workability of CRC. They also found that this treatment is more effective when the treatment time is longer. In addition, the compressive strength of the material could be increased by up to 3% simply by mixing the crumbs with dry cement before mixing them into concrete.

Performance Testing

In a further study, the UniSA and RMIT University researchers tested the relationship between the stress and the strain of different compositions of CRC when different percentages of sand were replaced with rubber. In solids, mechanical stress describes the forces that particles inside the material exert on each other when the solid is compressed or carrying a load. Strain describes how much the solid extends while under pressure. By measuring the stress-strain relationship of a material, physicists can reveal its 'elastic modulus' - a quantity describing a solid's resistance to being deformed. In addition, the 'toughness index' of a material quantifies how effectively it can absorb energy from impacts. For three different percentages of rubber mixed into CRC, the research team quantified the elastic modulus and toughness index, along with a mathematical description of the mechanical response of each material.

The team discovered that crumbed rubber generally decreases the compressive strength and elastic modulus of concrete. However, they also showed that CRC has a higher toughness index – when 18% of the material was composed of rubber crumbs, it became 11.8% tougher than traditional concrete. Using this data, the researchers developed several formulae to predict how the stress-strain relationship and elastic modulus of CRC will change with varying percentages of rubber. They



also constructed numerical models to predict this behaviour, which consistently agreed with their experimental results.

In their latest study, the team investigated the characteristics of the bond between CRC and steel profiled sheets. This bond is particularly important for structural applications in reinforced concrete, where the strength of concrete is greatly improved by networks of steel embedded in tensile regions. In smallscale tests, the researchers investigated the strength of the CRC-steel bond, noting that CRC had a similar performance to conventional concrete when bonding to steel. The difference in bond strength between the two materials was less than 4%. Their results confirm that CRC could indeed become a viable application for creating reinforced concrete slabs.

A Promising Future for CRC

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Through the work of the UniSA and RMIT University researchers, CRC now shows a promising potential, particularly for use in reinforced concrete. Using the team's insights to optimise the properties of CRC, it could allow for structures that can withstand impacts including bullets and debris in strong winds. Furthermore, the improved dynamic response of CRC could make structures able to better withstand events including earthquakes, machinery vibration and humaninduced vibration, making it an ideal material for constructing infrastructure, industry, and commercial and residential buildings.

In further research, the team plans to improve their numerical models to consider the technique of 'finite element analysis', which involves breaking down materials into small elements in a simulation. For any action applied to the material, the dynamics of each element is calculated individually, before the elements are integrated together, allowing the simulation to predict the dynamics of the material as a whole. Such improved models will allow the mechanical properties of CRC to be further optimised for commercial applications. With these improvements, an increased use of CRC in global construction shows promises to reduce the significant environmental impacts caused both from waste tyres and the exploitation of natural resources.

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Meet the researchers



Professor Julie Mills

Professor Julie Mills is Professor of Engineering Education, and Head of the School of Natural and Built Environments at the University of South Australia. Her diverse research interests include engineering education, gender studies and structural engineering. Professor Mills' current structural engineering research is focused on the use of recycled materials as partial aggregate replacement in concrete. She has authored numerous journal publications and coauthored two books.

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Associate Professor Rebecca Gravina

Associate Professor Rebecca Gravina is a Civil and Structural Engineer with 20 years of experience in academia and consulting engineering. Her current position is as Associate Professor in Civil Engineering at RMIT University, Melbourne. Professor Gravina received her PhD from the University of Adelaide and is now an established researcher with expertise in structural materials. She is also the Editor in Chief of the *Australian Journal of Civil Engineering*, and co-author of the book *Prestressed Concrete*. **E:** Rebecca.gravina@rmit.edu.au

Professor Yan Zhuge

Professor Yan Zhuge is a Professor in Structural Engineering, and has lectured in several Australian universities for more than 20 years. She has a PhD in Structural Engineering from Queensland University of Technology. Her main research interests include green construction materials, and sustainable concrete materials. Professor Zhuge has won several Australian and Queensland government awards. She is an executive committee member of the Concrete Institute of Australia.

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Dr Xing Ma

Dr Xing Ma has been involved in teaching and research in civil engineering for more than 15 years. He was a lecturer at Tongji University in China after he finished his PhD studies there in 2000, and was promoted to Associate Professor in 2004. Dr Ma joined the University of South Australia in 2010. His research is focused on composite structures and transmission tower structures. E: Xing.Ma@unisa.edu.au



Professor Bill Skinner

Professor Bill Skinner has spent over 30 years in surface science research, with 24 years in minerals processing. Since 1992, he has worked on physical and chemical processes at surfaces and interfaces at the University of South Australia. In particular, his research focuses on mineral and material surface chemistry together with forensics, environmental science and biomaterials. **E:** William.Skinner@unisa.edu.au









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CUCKOO SEARCH: USING EVOLUTIONARY ALGORITHMS TO OPTIMISE MATERIALS

From the metal in our cars to the circuits in our phones, the materials we use in our everyday lives can be meticulously engineered on a molecular scale to suit our requirements. However, there are so many possible arrangements of atoms and molecules at this scale that it is incredibly difficult for scientists to engineer materials optimised for the tasks they are designed to perform. **Dr Ganesh Balasubramanian** and his team at Lehigh University are working on solving this problem with help from an unlikely source of inspiration – the female cuckoo bird.

Graphene is a fairly simple-looking material on the face of it – carbon atoms arranged in a honeycomb lattice stretch out in a plane, forming a twodimensional carbon sheet with a vast range of possible applications. In reality, however, graphene tends not to be so orderly. Defects in graphene come in the form of extra atoms and molecules bonded to the sheet's surface or woven into the lattice, missing carbon atoms, and variations in carbon isotopes – forms of carbon atoms that have different numbers of neutrons in their nuclei.

Finding the Best Arrangement

Dr Ganesh Balasubramanian and his research team noticed that the effectiveness with which graphene carries heat – or its 'thermal conductivity' – can vary depending on the concentrations and distributions of different isotopes of carbon in the lattice. When certain arrangements of carbon-13 were present rather than pure carbon-12, the team found that the thermal conductivity could be greatly reduced due to enhanced scattering caused by vibrations in the lattice. Reducing this thermal conductivity would allow graphene to be used as a highly efficient insulator. Other applications could include sensors for high-frequency communication systems with little outside interference, as well as coatings for wires in analogue circuits, which would allow currents to be controlled more precisely.

The dilemma faced by Dr Balasubramanian and his colleagues was that the carbon-13 isotopes could be arranged in a vast variety of ways within the lattice, each of which reduced the thermal conductivity by varying amounts. The team needed a way to find the one optimal arrangement that would reduce thermal conductivity the most – a task that would take far too long should they test each arrangement one by one.

Dr Balasubramanian likens the search for an optimised material to buying a smart new shirt. 'We try it and if we like it, if it fits well, if it looks good on us, we think about buying it,' he explains. 'Even if we really like it but it doesn't fit us, we have to let it go or make a compromise. On the contrary, if we spend a little

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more, hire a tailor to select the fabric and stitch it according to our liking, the desired objective of being well-dressed is achieved.' With previous technology, the challenges faced by material engineers have been comparable to those of a tailor. 'We have to make tradeoffs when choosing the best material for the job – it may not have all the desired properties, but potentially checks the boxes on more items than a competing material,' he adds.

'The current state-of-the-art techniques are able to probe materials and subsequently predict and correlate relevant properties to the material composition and atomic structures. Thus, given a pure or engineered material, its properties can be measured and computed. But like with the tailor, this trial and error approach is expensive.' Dr Balasubramanian's team would need to use more sophisticated techniques to
'The basis of the method is derived from robust theoretical foundations of Darwin's natural evolution and habits of animal species like the Cuckoo bird. This approach enables us to compare numerous existing and hypothetical materials concurrently and to identify the best candidate for particular application.'



develop a graphene structure with an arrangement of isotopes that would optimally reduce thermal conductivity. They achieved this with an algorithm that uses the principles of Charles Darwin's theory of natural selection.

A Little Help from Darwin

Charles Darwin's elegant theory offers a watertight explanation of how species adapt and survive in the natural world. If two parents survive long enough to reproduce, their offspring will carry both of their successful characteristics on to the next generation, and the species improves as a whole. Occasional genetic mutations will sometimes improve the characteristics of offspring further, but will otherwise be swiftly bred out. Dr Balasubramanian and his team noticed how the foundations of this principle could be useful in establishing an algorithm that would help them with their graphene quandary.

Enter the genetic algorithm. In Dr Balasubramanian's study, an initial population consisted of simulated samples of graphene with different arrangements of carbon-13 isotopes. The genetic algorithm 'bred' these samples by creating subsequent generations of graphene samples that displayed isotope arrangements characteristic of their 'parent' samples. The prominence of each parent's arrangement in their offspring depended on how well it reduced thermal conductivity in graphene - comparable to how genetically favourable parents are more likely to pass on their traits. As the generations progressed, the team's algorithm introduced 'mutations' in the form of isotope arrangements, which were not present in any of the original samples. If these mutations proved to reduce thermal conductivity further, then the algorithm would pass them on to further generations - otherwise, they would soon disappear.

Using their genetic algorithm, Dr Balasubramanian's team managed to successfully engineer simulated graphene structures that were optimised to reduce thermal conductivity, which could prove invaluable when producing low thermal conductivity graphene in the lab. Over many generations, concentrations and distributions of carbon-13 isotopes that were less desirable gradually disappeared, until a material emerged that was optimised in displaying its desired property. However, the success of the algorithm would have its limits. In a later study, Dr Balasubramanian was faced with a new challenge in optimisation, which could not be easily solved using the elemental principles of natural selection.

An Elusive Secret Recipe

Metal alloys have vital and extensive applications in our everyday lives. Alloys containing just two metals are easy to optimise by fine-tuning the proportions of both elements until the properties of the material can no longer improve. However, throw more elements into the mix, and things become much more complicated. Alloys containing three metals can display properties that are more useful than those of simpler materials, but it is far more difficult to find the exact proportions of all three elements that will optimise a certain property. With four or five different metals, the task becomes virtually impossible.



Dr Balasubramanian and his team devised a method to tackle this challenge using more refined evolutionary principles.

In this study, the researchers simulated an alloy containing five separate elements. Depending on the proportions of each of the five elements used, the resistance of the alloy to breaking apart under tension – its tensile strength – can vary widely. The team wanted to find the perfect recipe to optimise tensile strength in the alloy, but even using their genetic algorithm, this would have taken far too much time and computing power. The team needed an even more sophisticated algorithm. To achieve this, his team's latest work would take inspiration from the evolutionary behaviour of one particular bird.

Nature's Most Reluctant Mother

The female cuckoo's instinctive disdain for devoted parenthood has driven her to a particularly devious egg-laying technique. She finds the nest of an altogether different species in which to lay her single egg, and never visits again. When the egg hatches, the cuckoo chick will push all of the other eggs from the nest, ensuring it has the undivided attention of the host mother. The trick is that cuckoos have evolved to lay eggs that realistically mimic those of other species. If the egg appears even slightly out of the ordinary to the host mother, she will either evict the egg from the nest, or build a new nest altogether. In evolutionary terms, the genetically sub-par eggs of the parent cuckoos would not then be passed on to the next generation.

The Cuckoo Search algorithm employed by Dr Balasubramanian's team exploits a similar technique. It selects groups of simulated alloy samples to act as the 'nests' of host mothers, and then plants a 'cuckoo' sample into the nest. If this new sample displays a higher tensile strength than the other eggs, the original nest of samples will be eliminated – comparable to how a successful cuckoo chick will evict the other eggs in its host nest.

The cuckoo sample will then be included in a nest of its own to be introduced to further cuckoo samples, and the process repeats. If tensile strength is not improved, however, the Cuckoo Search algorithm will eliminate the cuckoo sample, and the nest will pass on to the next generation, until an optimised sample is determined.

Overall, the team discovered that this algorithm could operate at a far greater efficiency than their genetic algorithm. 'This approach enables us to compare numerous existing and hypothetical materials concurrently and to identify the best candidate for particular application,' Dr Balasubramanian describes. 'Using the power of supercomputing, it drastically reduces the economic demands for such an exploration of the materials landscape, and accelerates the materials discovery process multi-fold.'

Now that his methods have been proved successful, Dr Balasubramanian hopes his team's research will have a strong influence on materials engineering in the future. 'The goal is to integrate feedback from materials synthesis and processing, and from the standpoint of scalable manufacturing to create a holistic tool for design and discovery of nextgeneration materials,' he says. 'These materials will potentially be derived from a combination of currently available ones and possessing an amalgamation of properties superior to what we presently have.'



Meet the researcher

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Dr Ganesh Balasubramanian completed his PhD in Engineering Mechanics at Virginia Tech in 2011. He then worked as a postdoctoral research associate in Theoretical Physical Chemistry at the Technical University of Darmstadt in Germany, before becoming a faculty in Mechanical Engineering at Iowa State University. Dr Balasubramanian entered his current position as Assistant Professor in the Department of Mechanical Engineering and Mechanics at Lehigh University in 2017, where he continues his multi-disciplinary research. He has a wide variety of research interests within engineering, ranging from nanoscale transport and mechanics, to advanced energy and structural materials. Some of his recognitions include the ASEE Outstanding New Mechanical Engineering Educator award, Summer Faculty Fellowships at the Air Force Research Lab, and the Young Engineering Fellowship from the Indian Institute of Science.

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COMPUTING & DATA SCIENCE

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COMPUTING & DATA SCIENCE

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COMPUTING: ENHANCING LIVES AND ENABLING SCIENTIFIC DISCOVERY

It's hard to think of something that has changed our lives so profoundly than computing. From healthcare to education, and from our jobs to our social lives, computing pervades almost every aspect of modern life.

As just one of numerous examples, computing has dramatically accelerated scientific advancement, particularly in the last two decades. From searching for scientific literature, to creating and analysing big data, and from simulating physical systems to enabling new modes of discovery, computing has become a central and indispensable part of the scientific method. Therefore, in this section of the edition, we celebrate the researchers who are spearheading the latest innovations in computing technology and data science.

In the first article of this section, we meet Dr Benjamin Jantzen and his team at Virginia Tech, who develop computer algorithms to help scientists understand how natural systems work. By making connections between data from different processes, the team's algorithms allow similarities to be observed where none have been noticed before, driving scientific discovery.

Also developing computational tools to gain meaningful information from datasets is Dr Rens van de Schoot at Utrecht University. Here, Dr van de Schoot explains how Bayesian estimation can be used to overcome the limitations associated with small sample sizes. This approach may prove extremely useful for scientists trying to learn about rare diseases, for which there is limited data. It may also be useful for predicting the development of symptoms in certain complex conditions.

Continuing on the theme of using computer modelling for accurate prediction, our next article introduces BreezoMeter – a company that develops algorithms to map and predict pollen levels. Breezometer's big data platform allows seasonal allergy sufferers to avoid areas that are forecast to have high pollen abundance.

Next, we showcase the work of Dr Ali Mesbah at the University of California at Berkeley, who also builds and improves computational models to more accurately predict random systems. Currently, the computer models we use to describe systems that change in random ways are often plagued with uncertainties. Using Dr Mesbah's approach, scientists can program their incomplete knowledge of a physical system into a computer model, and then allow the computer to gain information about it over time through real-time inputs from the system in question. This approach will lead to increasingly accurate models, facilitating scientific advancement.

From here, we shift our focus to new technologies that help computers systems cope with our rapidly increasing production of data. Here, we meet Dr Shikharesh Majumdar of Carleton University, who creates techniques for efficiently handling the analysis of large amounts of data and develops middleware platforms that unify geographically scattered computer systems. On the theme of accelerating scientific advancement, Dr Majumdar and his colleagues developed a system where software and hardware resources are linked together into a unified platform, which allows researchers to access data generated by experiments around the world.

Their work also has implications for improving the 'Internet-of-Things', where large numbers of independent objects communicate via the internet. In one study, Dr Majumdar described how a cloud-based system could be used to effectively manage large numbers of Internet-of-Things smart systems, such as sensors that monitor the condition of infrastructure or those that keep track of a patient's symptoms.

Although the Internet-of-Things holds the potential to dramatically enhance our lives in myriad ways, it does not come without its pitfalls. Because so much personal information is shared through the Internet-of-Things, maintaining data security is of utmost importance. Therefore, it is imperative that we strengthen our cyber-defence workforce.

Towards this aim, Dr Yier Jin of the University of Florida and Dr Cliff Zou of the University of Central Florida created cyberforensic.net – a website that aims to enrich the cybersecurity workforce by providing training in the areas of digital forensics and Internet-of-Things security. In the last article of this section, we showcase the team's efforts towards making their online digital forensics program available to many educational institutions across the US.

DYNAMICAL SYMMETRIES: DRAWING NEW CONNECTIONS BETWEEN NATURAL PROCESSES

Scientists throughout history have constructed rules that help them to understand how natural systems work, but their insights are often far from perfect. **Dr Benjamin Jantzen** at Virginia Tech has developed computer algorithms to help. By making connections between different processes that humans cannot pick up on, Dr Jantzen's algorithms allow similarities to be observed where none have been noticed before. This work could allow for applications including models of complex ecosystems and brain processes – explaining more accurately than ever before how large swarms of animals move.



Scientific Laws

As they gather results for their experiments, it is second nature for many scientists to use scientific laws - often first written out by their predecessor scientists - to describe what they observe. This system has clearly worked well for science so far, but Dr Benjamin Jantzen at Virginia Tech believes that even the brightest of human minds may not be intuitive enough to spot connections between some natural processes that initially appear unrelated. Ultimately, he thinks, we could be overlooking how different scientific processes that rely on entirely different sets of parameters could be displaying similar behaviours - an effect that could be well worth looking into for scientists.

'My group works on logical puzzles at the heart of science – puzzles about why and how the methods we bring to the laboratory or the theorist's notebook efficiently result in the sort of laws that let us predict and control natural phenomena,' Dr Jantzen says. 'One big question that drives a lot of our research is the problem of figuring out the collections of natural phenomena that are good candidates for scientific inquiry.'

Dr Jantzen believes that a more philosophical approach to exploring these collections of natural systems would afford scientists a far more in-depth understanding of the relationships between them. Through developing specialised algorithms, his team has focused on determining how seemingly arbitrary natural systems could be connected with more universal, previously unexplored sets of laws. This could help scientists to determine whether or not it would be useful for their research to explore connections that they hadn't previously considered.



Making Connections Between Processes

In their work, scientists often need to make decisions about how to group collections of natural processes into more all-encompassing theories. In doing this, they must choose how to distinguish between systems that can be grouped into categories that might share scientific laws and those that probably can't. It also creates issues for researchers when deciding which methods can be used to identify categories that are likely to be useful. 'We've built programs that can use data about the behaviour of two phenomena – like population growth in bacteria and in oak trees – to determine whether the phenomena are governed by the same "law".



Dr Jantzen describes the broad field of electricity as an example of a class of natural systems that past scientists decided were describable in terms of a single theory. 'Before anyone could build a theory about the behaviour of electricity, we had to decide which phenomena count as electrical,' he explains. 'Should we try to explain lightning the same way we explain why sparks leap off a wool blanket in the winter?' Ultimately, scientists in previous centuries decided intuitively that this was, indeed, a good idea.

This example shows that in constructing all-encompassing fields such as electricity, scientists are capable of using their own logic to decide how to group individual natural systems into categories governed by a single law – provided they can spot connections between theories describing each individual system. However, this way of thinking doesn't address the issue of devising robust methods for grouping together natural phenomena that appear to be unrelated.

To solve this issue, Dr Jantzen proposes a shift in thinking, to comparing the 'dynamical symmetries' of systems that are seemingly unrelated in their behaviour. 'Think about the behaviours of two springs with shock absorbers,' he says. 'Each spring exhibits very different behaviour - one bouncing up and down all day long, the other smoothly reaching equilibrium. But underneath their differing behaviours is a shared equation of motion. By directly detecting that they share such an equation, you can see right through different behaviours without learning their governing laws first.'

This example shows how dynamical symmetries can describe a pattern in the way features of a system relate to one another, rather than the features themselves. By accounting for and comparing dynamical symmetries through specialised algorithms, scientists would be able to spot connections between natural processes for the first time.

A Step Up from Machine Learning

Scientists commonly use 'machine learning' algorithms to predict outcomes in natural systems. These algorithms base their predictions on the assumption that the system of interest is passively observed. 'Machine learning algorithms can learn, for example, to predict when the lights will be on, given the positions of the light switches,' Dr Jantzen explains. However, it is often more useful to know what will happen when we interact with a system. 'In general, these algorithms can't tell you what to do to the light switches in order to make the lights come on.' Dr Jantzen's team aimed to improve on these methods by creating algorithms that learn the 'what-ifs', allowing them to predict what would happen if a system were changed.

'Our methods are very different from the sort of assessments or predictions one can make with most machine learning tools,' Dr Jantzen continues. 'My group has begun to understand some features





of those collections of things that can be usefully described by scientific laws, and we've built computer algorithms that can detect these features automatically. That is, we've built programs that can use data about the behaviour of two phenomena – like population growth in bacteria and in oak trees – to determine whether the phenomena are governed by the same "law".

With these methods, Dr Jantzen's team has already created algorithms that allow them to identify dynamical symmetries of two different systems, revealing new ways to group natural systems together. 'As opposed to machine learning, our algorithms tell us whether two phenomena have a similar causal structure – in other words, whether they are governed by the same laws that determine how one property changes, given changes in the others, even if we have no idea what those laws are,' he says.

Predicting Swarming Behaviour

Using advanced algorithms, Dr Jantzen's team, in collaboration with Dr Nicole Abaid at Virginia Tech, has already demonstrated how uncovering dynamical symmetries between seeminglyunrelated natural systems can be remarkably useful for a variety of applications. Systems ranging from complex networks of computer models or brain signals, to behaviours and interactions between different wild species, are all examples of phenomena whose hidden structure can be compared through dynamical symmetries.

'Such algorithms are of enormous practical value,' says Dr Jantzen. 'We're using our algorithms to test the validity of complex computer simulations, to figure out how many expensive field measurements are needed in order to accurately model an at-risk ecosystem and have even begun to sort complex brain processes according to their hidden, underlying laws.'

Yet perhaps the most intriguing application of Dr Jantzen and Dr Abaid's work involves significant improvements in predictions of how animals in large swarms – behaviour that is seen across a wide variety of species – will move.



Previous studies on swarming behaviour, typically relying on much more simplistic algorithms, have managed to roughly approximate the superficial behaviour of swarms, but have struggled to precisely model swarm movements as a whole based on the movements of individual animals. By using realworld observations as inputs into their algorithms, Dr Jantzen, Dr Abaid and their colleagues have managed to greatly reduce this problem.

'A swarm of bats has its own dynamical symmetries, distinct from those of a bat by itself,' Dr Jantzen explains. 'But there is a connection. The bat swarm is made up of bats, so if its dynamics is different from a bird flock, we know that the individual bats must be doing something different to individual birds.'

'Using these principles, the researchers are now studying computer simulations that accurately predict swarming behaviours. 'We're using our discovery algorithms on video data to sort collective behaviour in organisms based on the unknown laws that govern how such swarms of animals operate. No one has done this in a quantitative way before,' Dr Jantzen continues. 'We're also using our algorithms in a slightly different way to test whether any of the existing models of collective behaviour – which can generate convincing simulations on the computer – actually reflect the mechanisms driving animal swarms.'

From a seemingly philosophical starting point, based on questioning how scientists can decide how to group individual natural phenomena together, Dr Jantzen's team has already offered innovative solutions to long-standing scientific problems. 'Far from a purely academic exercise, our work on logical problems of scientific discovery is finding application in multiple fields,' he concludes.

In the future, not only scientists, but those in a wide variety of other fields could look to algorithms that account for dynamical symmetry to provide new insights into their work – leaving computer calculations to spot the elusive connections that human minds haven't yet been able to see.

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Meet the researcher

Dr Benjamin Jantzen Philosophy Department Virginia Tech Blacksburg, VA USA

Dr Benjamin Jantzen holds graduate degrees in both physics and philosophy, and a doctorate in Logic, Computation, and Methodology from Carnegie Mellon University. Currently, he is an Associate Professor of Philosophy at Virginia Tech. Here, his interdisciplinary research is focused on the development of computer algorithms for scientific discovery and on the philosophical impact of these algorithms on our understanding of the world and ourselves. With an NSF CAREER Award, 'Automated scientific discovery and the philosophical problem of natural kinds', Dr Jantzen is leading a diverse team using philosophically motivated tools of discovery to learn about everything from bat swarms to brain scans. He is also the director of an annual workshop called 'Philosophy & Physical Computing', which is aimed at providing philosophers, computer scientists, and experimental scientists with the technical skills and philosophical perspective necessary to collaborate with one another on problems of common interest.

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STATISTICAL METHODS FOR SMALL DATA

Researchers are heavily reliant on statistical techniques that are based on large sample sizes. Therefore, attempts to gain useful information from small samples can often lead to biased, or incorrect conclusions. **Dr Rens van de Schoot** at Utrecht University has shown that the limitations associated with small samples sizes can be overcome by using an alternative method – Bayesian estimation – as an all-encompassing approach to quantitative research. However, this approach comes at a price: expert knowledge must be integrated into the statistical model.

Beyond Coin Toss Statistics

In statistics, sample sizes have traditionally played a large role in the knowledge we can derive from a given field. By testing a large number of different instances of a phenomenon, we increase the likelihood that the results achieved are an accurate reflection of reality. Analogously, by flipping a coin endlessly, we can continually refine the data we have about the likelihood of an outcome.

This 'tossing a coin' approach to statistics is called the frequentist paradigm, and one that Dr Rens van de Schoot of Utrecht University has been working to overhaul. With his recent research on Bayesian methods to deal with small sample sizes, he has been working to challenge the reliance of statistics on mere numbers.

'I mostly work on small sample size problems,' Dr van de Schoot explains. 'For example, there are few children with burn wounds, that it's hard to do any representative statistical analysis on them. For those kinds of topics, I look for the appropriate statistical methods for such cases. Then I find, for example, the clinicians treating such victims, and who would benefit from such statistical methods.' Because researchers rely so heavily on techniques based on large sample sizes, limitations associated with the samples available can restrict the usefulness of the data obtained. Dr van de Schoot explains that researchers may suffer from small sample sizes because large ones are scarce, subject to bureaucratic barriers, or costly, as with studying children with severe burn wounds, for example.

Researchers can circumvent small sample sizes through simplifying their hypotheses or statistical models, but the limitation inherently tends to produce biased results in analyses. The skewed results produced are therefore less in line with the greater context of the field, and don't take full advantage of human knowledge as a whole.

Maximum likelihood estimation is a method that seeks to find the most plausible parameters of a statistical model. In a 2015 study, by Dr van de Schoot and his colleagues demonstrated that this estimation technique results in biased findings if sample sizes are small. This is because it is based on the central limit theorem – it only provides reliable results with many data, just like in the coin toss example.





Dr van de Schoot and his team also showed that the reliance on a large amount of data can be overcome by using an alternative method – Bayesian estimation – as a more allencompassing approach to quantitative research. But it comes with a price: expert knowledge must be integrated into the statistical model. 'I am a project initiator: I jump on innovative ideas on knowledge production and build bridges between the right types of knowledge and people to make these ideas a reality. Because of my optimism and energy, I enjoy motiving colleagues to strive for a common goal.'



A New Paradigm in Statistics

Dr van de Schoot has drawn attention to the fact that there is increasing recent interest in Bayesian statistics and analysis in, for example, psychology, educational research and posttraumatic stress.

Developed in the 18th century, Bayesian statistical methods have recently become more common in social and behavioural science research. The Bayesian paradigm offers a different view of interpreting probability as a subjective result of uncertainty. This statistical approach involves the incorporation of background knowledge from previous studies, using as much previous information as possible in combination with personal judgment by experts. The combination of previous knowledge plus new findings provides an updated view of 'plausibility', producing a view of which strategies in the given field could move.

There are three ingredients of Bayesian statistics. The first is the background knowledge, which reflects levels of pre-existing knowledge including the uncertainty attached to it. This background knowledge is then translated into a statistical distribution, called the prior distribution. The second component is the data from the research itself - this is expressed as 'likelihood'. The third component is posterior inference, which combines the first two aspects under the Bayesian theorem. It is a compromise, as it reflects updated knowledge but is balanced by observed data. For this reason, Dr van de Schoot argues that Bayesian statistical methods are unique in their capacity to produce a cumulative form of knowledge.

The background knowledge used in Bayesian analysis often comes from systematic reviews, meta-analyses, previous studies on similar datasets, or even experts. Dr van de Schoot argues that having background knowledge as part of the statistical model is particularly important in psychology, because prior research has established that replication is a crucial tool in the field.

Bayesian statistics allow past work to be built on in a meaningful way. The technique helps to better contextualise research data, creating results with a more all-encompassing view. Because background knowledge also contains information, it can be viewed as, loosely formulated, additional data, which is used in the estimation of the statistical model. As a result, large sample sizes are not necessarily needed in Bayesian statistics, putting less restrictions on the size of the datasets. So, Bayesian estimation can use smaller samples while demonstrating greater power of prediction due to its incorporation of prior distributions.

However, Dr van de Schoot warns that 'researchers should not use such methods because they are lazy and don't want to collect more data, but only if collecting data is simply not possible for whatever reason.' This is the case for the data available on post-traumatic stress, which is one focus of Dr van de Schoot's recent research.

Dr van de Schoot's aim in his recent work into the development of post-traumatic stress symptoms after a traumatic experience is to investigate how much background information is needed to overcome small data issues, find where to get it, how to elicit it, and how to report the whole process.

Anticipating the Effects of Trauma

Previous work highlights that after traumatic events, approximately 10% of individuals develop post-traumatic stress symptoms. Some symptoms may persist for years and can have profound negative effects on a sufferer's life, including medical bills, work absence and substance abuse. When post-traumatic stress is overlooked in the early stages, it can have particularly harmful long-term effects. It is therefore of significant social importance to understand the trajectories that post-traumatic stress disorder can take.

Dr van de Schoot refers to research from 2004 by Dr George Bonanno of Columbia University, in which two relatively stable patterns of post-traumatic stress development and two more dynamic patterns were identified. *Resilient and chronic* trajectories were more simply accounted for in this study, whereas a decreasing recovery and an increasing 'delayed onset' trajectory were more variable.

Most studies that have been conducted since then support these four distinctive trajectories. However, Dr van de Schoot and colleagues point out that the 34 papers produced since the cornerstone 2004 study all employed a technique that is not statistically equipped to detect smaller trajectories such as delayed onset. They state that this does not produce a sufficiently comprehensive picture of the numbers suffering from certain conditions.

The chronic trajectory and delayed onset trajectory only exist to a small extent in the data results. Because delayed onset trajectory sufferers generally present symptoms only after the limited period in which resources such as hospital treatment and legal support are available, their condition may not be identified or treated. Additionally, these symptom patterns often reach a high level of severity. This is why, Dr van de Schoot and his colleagues argue, it is necessary to develop models using statistical methods that are sensitive to smaller quantities of data (i.e. Bayesian statistics with background information incorporated into the analyses). Only these would have the sophistication to predict the development of such symptoms. 'The awareness that small but clinically relevant trajectories may appear, even beyond the acute phase, may help clinicians to develop efficient follow-up programs and to provide these individuals with help when indicated,' says Dr van de Schoot.



Statistics for the Future

The 2004 study in which four distinct trajectories were found for post-traumatic stress symptoms after a traumatic experience is a site that Dr van de Schoot feels is necessary to re-examine under the lens of Bayesian statistics. He aims to re-analyse the datasets created by the 34 studies that have been published since. By creating new and more macrocosmic data, he hopes to institutionalise a more broadly encompassing model with which further studies can be undertaken.

Dr van de Schoot sees the future of this statistical technique as only being enhanced as the Information Age progresses. He notes that Bayesian computational methods are increasingly available in free and proprietary software, and argues that this means researchers using statistics should not have reservations about taking advantage of this new paradigm. 'I want to create a workflow between field experts and statistical experts to help each other get more understanding,' Dr van de Schoot states. 'What gives me most joy is that society as a whole eventually benefits from this exchange of knowledge.'

In time, Dr van de Schoot hopes that experts, data scientists, professionals and individual researchers will no longer need to be rendered separate from each other through isolated research practices, and that information can be synergised in a meaningful way through which ordinary members of society can directly benefit. With these new techniques at researchers' disposal, he believes in the power of Bayesian analysis to provide them with more powerful tools for interdisciplinary action that benefits previously discrete fields mutually. This could lead to conclusions and understandings that existing methods have not readily accommodated.

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Meet the researcher

Dr Rens van de Schoot Utrecht University Utrecht The Netherlands

Dr Rens van de Schoot obtained his PhD from the Methodology and Statistics Department at Utrecht University in 2010, graduating cum laude and winning the APA award for best dissertation of the division of Qualitative and Quantitative Methods. Directly after achieving his PhD, he was appointed as Assistant Professor at Utrecht University, where he is now an Associate Professor. Here, Dr van de Schoot primarily conducts research into Statistics for Small Data Sets, Bayesian statistics, responsible research practices and posttraumatic stress disorder. He is a member of the Young Academy of The Royal Netherlands Academy of Arts and Sciences (KNAW), a member of the program board of the think-tank called the FD young circle, and has recently become a member of The Society of Multivariate Experimental Psychology (SMEP). Dr van de Schoot also works as a statistical research consultant for the many organisations such as the Association of Dutch Burns Centres (VSBN), and the Netherlands Centre for Graduate and Research Schools in The Netherlands.

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MAPPING ALLERGIES: A MODERN APPROACH TO POLLEN PREVALENCE REPORTING

For seasonal allergy sufferers, the warm spring weather that delights most comes with unpleasant symptoms and breathing difficulties. However, most methods of predicting pollen abundance are not precise enough to help the afflicted avoid high pollen areas. BreezoMeter is a bold young company that has made waves using big data innovations to change how we look at and understand <u>pollen data</u> and air pollution.

Painful sinus headaches, itchy eyes and struggling to breathe through a congested nose - for millions of people worldwide, seasonal allergies due to pollen are an unfortunate reality. In the United States alone, the Centers for Disease Control and Prevention estimates that the afflicted spend \$18 billion every year on allergy medications to keep symptoms at bay. For those with more serious sensitivities such as asthma, high pollen counts can increase the risk of a medical emergency. When combined with air pollution, high pollen levels add to a perfect storm of irritants that reduce allergic people's quality of life and increase their risk of health complications.

BreezoMeter is an innovative company that has transformed how air quality is reported and understood worldwide. Their big data platform uses proprietary algorithms that use measurements from government monitoring stations, meteorological, satellite and traffic data, to create comprehensive, <u>real-time air</u> <u>quality maps</u> of air pollution around the globe. BreezoMeter's technology can describe air quality variation with precision down to a city block, providing health conscious users with recommendations and predictions for outdoor activities in areas that will allow them to breathe easy. After years of significant research, development and investment on the back of increased industry demand, the company is now providing locationbased pollen levels. This key component of air quality has previously not received the same level of monitoring as pollution has in most countries, despite affecting millions of people's health.

The Problem with Pollen

Pollen grains are the male reproductive cells of plants, which are emitted by flowers in the hope that they will find and fertilise another flower of the same species. These pollen grains can either be transported through the wind or on the bodies of insect pollinators.

People that are allergic to pollen are most commonly affected by the pollen of plants that adopt a wind pollination strategy. Many trees and grasses use this tactic, producing massive amounts



of pollen to compensate for a mode of transmission that is not particularly accurate and relies heavily on luck. Anyone living in an area with abundant evergreen trees or grassland has probably enjoyed the experience of finding their car coated in the powdery yellow substance when the weather starts to warm up.

Pollen season is defined as the periods that these plants release pollen in a given region, and typically varies from year to year depending on environmental factors, such as temperature, rainfall, and day length. People with pollen allergies experience a range of near-constant symptoms



during pollen seasons, often known as seasonal allergies or hay fever. These allergies are common, with a prevalence of over 10% in many industrialised nations, including <u>67 million</u> seasonal allergy sufferers in the US alone, but their origins are not fully understood. Another challenge with pollen is that it can affect people's health immediately after exposure. In fact, one study found that even short-term exposure to a modest elevation in pollen levels (17.6 grains per cubic metre) increased the incidence of asthma attacks by 54%. There is likely a genetic component - however, there also appears to be a large environmental component. Pollen allergy rates are much higher in urban areas, and some researchers predict that airway irritation due to urban air pollution may be a contributing factor to the development of pollen sensitivity.

Those with pollen sensitivities are also usually sensitive to air quality as a whole and are in for particularly bad symptoms when both pollution and pollen rates are high. This mixture can be deadly for asthma sufferers, or people with similar respiratory problems. Even for those without specific pollen allergies, air pollution drastically impacts health and the higher particulate burden in the air can act as an irritant.

Air Quality Quagmire

Understanding air quality fluctuations is important but can be difficult under ever changing conditions. To further complicate the tracking of seasonal air quality, climate change is playing a role in shifting pollen seasons for many of the major airborne pollen producing plants. Many plants responsible for some of the worst seasonal allergies, such as ragweed, are thriving in the heightened atmospheric carbon dioxide concentrations associated with climate change.

Studies investigating both ragweed and loblolly pine have found that these plants produce 132% more pollen at current carbon dioxide levels than pre-industrialisation levels and this is expected to increase as concentrations continue to rise. Some experts predict that pollen levels will have fully doubled from current counts by 2040, meaning greater suffering for those with allergies. In addition to producing more pollen, many plants are flowering over longer periods of time, increasing both the length and severity of pollen seasons, particularly in climates where a winter to spring transition occurs. Despite the role of pollen in human health and environmental quality, it is typically not well monitored by the majority of world governments. As a natural phenomenon, pollen often garners less attention than sources such as car and factory emissions, which can be more easily controlled by government regulations. Since pollen does not affect everyone and is not present all year round, there is also a perception among many government officials that pollen is a fleeting concern that does not carry enough impact to warrant tracking.

However, pollen allergies are on the rise, particularly in urban areas, and an increasing number of people are expressing interest in knowing when pollen levels will impact their health and the health of their families. For those with pollen sensitivities, particularly asthma, awareness of current air quality measures that include pollen



rates could help them plan happy, healthy outdoor activities accordingly. BreezoMeter is working to make this a reality for allergy sufferers around the world.

Changing the Pollen Data Landscape

One of the greatest barriers to obtaining accurate pollen counts in a timely manner is the time and labour-intensive nature of most methods of pollen quantification. Currently, most major cities that track pollen do so using pollen counting stations. Of the cities that have some sort of pollen monitoring program, most only have one station. These stations operate a volumetric air pump – a machine that moves air over sticky films over a 24-hour period, catching any airborne particles. After 24 hours, a laboratory technician uses chemical stains to makes slides of the caught particles, and a certified pollen identification specialist then uses a microscope to count a subset of all pollen types on each slide, depending on the specialist's ability to recognise different species.

This means that standard counts are often delayed and rely upon numerous highly trained individuals to interpret. This is why many countries do not perform comprehensive pollen sampling across short timescales. In places that do perform measurements, pollen counts are often performed only on weekdays or once a week and are generalised over a large area. However, much like air pollution, changing local conditions can create pockets of heavy pollen that change quickly during the day or are moved to other areas by weather patterns.

In Europe, BreezoMeter bases its pollen reports on the European Union's Copernicus Atmosphere Monitoring Service (CAMS) to combine pollen predictions with big data in order to depict how and when pollen will move across different areas on a fine scale. BreezoMeter integrates CAMS models with their algorithm, which combines information that estimates where pollen will originate and describe its movement through the air. The CAMS model captures interactions between land use and weather movements to predict where pollen will stay airborne and where it will accumulate on land, while also predicting how air moves across different grids of an area. Also incorporated in the model is how different kinds of pollen flow in airstreams. When combined with the EU CAMS pollen forecasts, BreezoMeter's algorithms depict how pollen is moving across Europe in high detail. This information is translated into a simple pollen count index (PCI) of low, medium, high and very high, allowing allergy sufferers to easily check where they are most likely to be able to enjoy symptom-free activities. PCIs are based on the number of pollen grains in a cubic meter of air, and BreezoMeter provides regionally specific definitions for the areas the company operates. In Europe, the PCI integrates pollen indexes from multiple countries, accounting for plant species present and their likelihood to cause health effects.

Next Generation Pollen Counts

Leveraging novel pollen counts collected by the Japanese government, BreezoMeter is using technology and big data to transform how pollen is reported on a grand scale. Rather than relying on manual counting, Japan has installed hundreds of high-tech automatic pollen-counting sensors throughout the country.

These small stations rely on novel technology to provide realtime pollen identification and counts. Tiny streams of air are pumped through the machines and blasted with a beam of light. Sensors capture the characteristics of the light bouncing off the particles, and algorithms quickly identify if the sample is pollen. These results are further validated by Japan's air quality authorities using traditional methods. In Japan, the PCI is determined by the Tokyo Metropolitan Institute of Public Health using simple and intuitive pollen parameters.

BreezoMeter's algorithms receive fine scale input as conditions change and constantly adjust their output based on real-time data. With this vast and timely data source, pollen maps are very responsive to sudden changes and are able to update on an hourly basis. Seasonal allergy sufferers in Japan can see where they'll encounter pollen with incredible accuracy.



Changing the Game for Allergy Sufferers

BreezoMeter's big data approach to pollen forecasting is completely transforming how governments, corporations and individuals interact with pollen data. With up-to-date, location-based pollen data, those with severe sensitivities for whom pollen can be dangerous, such as people with asthma, can now enjoy outdoor activities when they know pollen levels are low. BreezoMeter's technology allows them to be aware and prepared on days where pollen activity could cause them harm.

Governments and corporations can identify areas that would benefit from increased air filtration systems and adjust strategies to match seasonal changes. Unlike traditional monitoring systems that provide broad regional measurements with a 24-hour delay, BreezoMeter is able to provide hourly pollen abundance data with a resolution of 250 to 500 metres. This allows people that suffer from allergies to make informed decisions that can improve their health and quality of life. Using BreezoMeter's hourly pollen data, people can decide when they should go outside, and where they should do their outdoor activities.

BreezoMeter's pollen modelling is even more powerful when combined with the company's proprietary air pollution algorithms, providing a comprehensive and fine scale map of air quality that captures the full picture of factors.

Founded in 2014 when a small group of environmental and software engineers came together to address the problem of how they could find healthy, clean places to live, considering that some of their family members suffered from respiratory diseases, the company is driven by a commitment to helping people live healthier lives through cleaner environments. Their simpleto-integrate API allows businesses to integrate air pollution and pollen data for commercial use, to develop better air purifiers, connected medical devices, smart homes, and lifestyle products that help people breathe easier worldwide.

About BreezoMeter

BreezoMeter is the world's leader in location-based, realtime air quality and pollen data, covering more than 5.5 billion people worldwide in more than 80 countries, and improving health by providing intuitive and actionable data. Using governmental sensors, satellites, local weather, transportation dynamics and other sources, BreezoMeter gives companies the tools to increase user engagement and sales, and impacts lives with accurate data, including pollen levels, pollutant concentrations and forecast. BreezoMeter offers its data via API to enterprises of diverse industries, including smart homes, air purifiers and HVAC, fitness and lifestyle, cosmetics, automotive, and medical device and health technologies.

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LEARNING-BASED PERFORMANCE OPTIMISATION OF UNCERTAIN SYSTEMS

Many systems in nature change in random, unpredictable ways over time. From the motions of microscopic particles in fluids to the daily price of stocks, random processes play a large role in systems we interact with every day. Also, because of our incomplete understanding of the phenomena underlying many non-random systems, the mathematical models we use to describe them are often plagued with random uncertainties. **Dr Ali Mesbah** at the University of California at Berkeley aims to optimise the performance of random and uncertain systems through learning their behaviour in real time.



Stochastic Systems

Random, or 'stochastic' systems present an intriguing problem for mathematicians and physicists. The term describes how the dynamics of a variety of both natural and humanmade systems can often depend on collections of variables that are ultimately arbitrary. It can also arise in mathematical descriptions of non-random systems due to their own random uncertainties. In these cases, it becomes difficult to predict how properties of these systems will change and progress over time. Dr Ali Mesbah and his team at the University of California are interested in stochastic systems that exhibit 'nonlinear' behaviour, where changes in the input of the system are not necessarily proportional to changes in the output.

Stochastic nonlinear systems encompass a variety of processes that require high degrees of control, from the molecular interactions in selforganising or biological systems to energy efficient buildings. By building and improving mathematical models to approximate their behaviour, researchers are beginning to describe them with increasing accuracy – giving the user controlling a system a say in how it will progress, and in how its behaviour can be optimised to their specific requirements. However, many researchers have found simulation and performance optimisation of stochastic nonlinear systems to be a challenging task.

Optimisation under Uncertainty

When attempting to control stochastic systems, researchers are ultimately faced with two fundamental challenges. The first of these is the enormous complexity required for models to accurately reproduce the behaviours of physical systems inside a computer. When building models that are based



upon the most fundamental laws of physics, researchers will need to account for an increasingly intricate web of physical, chemical and/or biological phenomena to ensure their simulations remain accurate.

Secondly, our understanding of the fundamental laws of physics themselves is far from complete. This means that when researchers program these laws into their models, they also need to program in the uncertainties



associated with the laws – creating an inherent uncertainty in the overall model. Together, these issues pose key challenges to performance optimisation of complex systems.

The overreaching objective of Dr Mesbah's research is to develop learning-based approaches to addressing the performance optimisation of uncertain, complex systems. Starting from programming our incomplete knowledge of physical laws into computer models, this approach would allow computers to gain information about the laws over time – allowing them to reproduce system behaviours with increasing accuracy.

For researchers, this approach would ensure that their operations on physical systems remain safe and reliable, even in the face of uncertainties. Dr Mesbah is investigating how this innovative approach for solving learning-based optimisation of uncertain systems could be implemented in practice.

Control Through Learning

Mathematical approximations of systems are commonly used in physics to explore their general trends, rather than precisely predicting their behaviours. By defining relatively simple sets of equations, researchers can describe generally how systems behave, without the need for implementing tedious fundamental laws and uncertainties into their models.

This level of detail isn't sufficient for performance optimisation of complex systems in itself, but Dr Mesbah proposes that approximations can serve as a baseline that real-time models can continually refer back to. By 'learning' about how a system behaves in real time, this approximate model can be continually updated to more accurately reflect the real system. Using an approximation of a system as a solid baseline in performance optimisation ensures that the performance of a controlled system remains stable and reliable in the face of uncertainties. Meanwhile, the system's performance can be optimised based on the updated knowledge (or model) of the system. 9)

In addition to approximate models, Dr Mesbah proposes that high-fidelity models of systems can be used to continually verify the performance of controlled systems. By referring back to these models, a controlled system's performance can be updated if necessary, and the process can repeat.

Dr Mesbah has recently explored the technique of 'Model Predictive Control' (MPC) – an optimisation-based control method that relies upon satisfying a particular set of constraints. For several decades, this method has been widely used as a solution in optimal decision making in constrained systems with many variables. Currently, its applications range from manufacturing and chemical processing, to path planning for unmanned vehicles. However, until now, MPC has not been



seen as an effective tool to address optimal control through active learning.

In his latest research, Dr Mesbah and his colleagues have explored how probing MPC-controlled systems can reduce uncertainties in system models. By generating input and output data on the closed-loop control loop, more information can be gathered about the real-time operation of the system – addressing the long-standing question of how MPC can be used to realise active learning.

In particular, the team focused on how incorporating probing in the control action could reduce uncertainties in the predictive capability of a model relevant to performance optimisation under uncertainty. Ultimately, the team's study demonstrated the potential of active learning for maintaining MPC performance, even in the face of uncertainties in the model's parameters and overall structure. The study revealed that active learning is particularly beneficial when a system undergoes abrupt changes – maintaining its safety, reliability, and profitability. Dr Mesbah believes that these advantages would prove particularly useful in one fascinating application.

Controlling Atmospheric Pressure Plasma Jets

Plasma may be one of the most extreme states of matter we currently know about, but its properties can still be remarkably useful to us, particularly in materials processing and medical applications. Composed of a 'soup' of hot, unbound positivelyand negatively-charged ions, plasma can be generated in a variety of interesting ways. One of these is the Atmospheric Pressure Plasma Jet (APPJ) – an intensive stream of plasma ions ejected from a handheld nozzle, with a pressure that matches that of the surrounding atmosphere, enabling high degrees of control in environments outside the lab.

Within APPJs, the motions of ions represent a key example of a stochastic nonlinear system. Many different variables affect how the dynamics of the system evolve over time, including the charges of the ions, their temperature, and the speed at which they are ejected. Using conventional feedback control methods, it would be virtually impossible to control the system in a way that could bring about perfectly optimised results.

Dr Mesbah's team aims to address this issue by using their MPC technique to control APPJs – taking real-time system measurements and combining them with a model of the system to determine optimal inputs of the system. This ultimately allows the performance of APPJ systems to be optimised to the performance requirements of their users. By adapting the model for the specific case of describing jet dynamics, the team has now given users of APPJs control over the systems for the first time.

Targeted Delivery of Medical Treatments

Dr Mesbah's recent research has resulted in new strategies for enabling safe and effective dose delivery in biomedical applications of APPJs. APPJs are an ideal candidate for delivering small doses of chemical, thermal and electrical treatments to specific targets without the need for more invasive treatments. However, researchers attempting this technique have previously faced challenges in constraining APPJs within a safe operating region – as stochastic nonlinear systems, it remains difficult to gain optimal levels of control needed to operate the jets. Delivering a dose to the wrong region, or in the wrong amount, could have dangerous consequences for a patient.

In several recent studies, Dr Mesbah and his colleagues have explored how MPC strategies can be used to control APPJs in situations that mimic medical treatments. They demonstrated how by carefully controlling how much of a dose is being delivered and accumulated to a specific region over time, input parameters on the jet can be continually adjusted to account for changes in the dynamics of the jet.

Through simulations and experiments, Dr Mesbah's team has shown that MPC strategies could provide a versatile method for delivering targeted doses safely, consistently and effectively. Even for a nonlinear system such as a plasma jet, the technique would remain reliable in the presence of the wide variety of disturbances that can occur inside the body, while also accounting for human errors such as the distance between the handheld APPJ nozzle and the target tissue.

Reliable and therapeutically effective control of APPJs will lead to significant progress for medicines that can accomplish feats including shrinking cancerous tumours and increasing healing rates in chronic wounds. Perhaps most intriguingly, it could enable the development of APPJs that can deactivate antibiotic-resistant bacteria – potentially a critical step forward for one of the most urgent areas of modern medicine.



Meet the researcher

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Dr Ali Mesbah is Assistant Professor of Chemical and Biomolecular Engineering at the University of California at Berkeley. Before joining UC Berkeley, he was a senior postdoctoral associate at MIT. He holds a PhD in systems and control from Delft University of Technology and is a senior member of the IEEE Control Systems Society and the American Institute of Chemical Engineers (AIChE). He is the recipient of the AIChE's 35 Under 35 Award in 2017, the IEEE Control Systems Outstanding Paper Award in 2017, and the AIChE-CAST W. David Smith, Jr. Publication Award in 2015. His research interests are in the areas of optimisation-based systems analysis, fault diagnosis, and predictive control of uncertain systems.

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IMPROVING HIGH PERFORMANCE DATA ANALYTICS PLATFORMS & SMART SYSTEMS: RESOURCE MANAGEMENT AND MIDDLEWARE

Our rapidly increasing production of data is straining computer infrastructures to unprecedented levels. As researchers develop much-needed coping mechanisms, **Dr Shikharesh Majumdar** at Carleton University focuses on two important solutions to the issue: creating techniques for efficiently handling the analysis of large amounts of data and developing middleware platforms that unify geographically scattered computer and storage resources.

According to IBM, the amount of data we generate every day now exceeds a staggering <u>2.5 quintillion bytes</u>. As this figure increases unrelentingly, the current infrastructures in place to deal with this information are becoming increasingly strained. The world of technology is now faced with key challenges in making sense of the sheer amount of data and extracting useful information from it. As Dr Shikharesh Majumdar of Carleton University explains, these challenges stem from what he refers to as the well-known '3V characteristics' of Big Data.

The first 'V' refers to the 'volume' of data, which describes the extremely large size of the information being produced. The second 'V' stands for 'velocity', which is important when describing flows of information, in contexts ranging from Twitter feeds, to sensor data streams in sensor-based smart systems that include buildings, bridges and machinery. Finally, 'variety' refers to the different types of data that are produced, in forms including text, images, and numbers.

In his research, Dr Majumdar aims to address these challenges in two critically important areas of data handling. Both areas have involved developing new types of 'middleware' – a type of software that bridges the gap between an operating system and its applications – for effective resource management. One area involves creating resource management techniques that allow large-scale data processing platforms to operate at a high performance. The other focuses on middleware that unifies various resources scattered over multiple locations, for managing sensor-based smart systems.

Over the last few years, Dr Majumdar and his colleagues have addressed a variety of the issues involved in each area. Research in the first has led to a novel resource management algorithm, which resulted in an article in IEEE Transactions on Parallel and Distributed Systems [2], one of the premier journals in the field, and another paper that received the best paper award at a reputed IEEE International Conference. Dr Majumdar and his team's pioneering R&D work in the second area has produced a platform for research collaboration among researchers of smart facility management, described by the Canadian Network for the Advancement of Research, Industry and Education (CANARIE) as: 'first of its kind, it allows geographically dispersed researchers to share data-analysis tools, sensor data, and expertise to manage smart facilities'.



Managing Resources on Big Data Processing Platforms

Today, many data storage and processing resources are provided by cloud and cluster-based platforms, which link many systems together to share information. These systems are fundamentally important to many different users, from businesses and financial institutions to researchers and engineers, who will often generate large amounts of data.

Among the achievements of Dr Majumdar and his colleagues in this field is in resource management for batch data analytics platforms, which allows for techniques that allocate computer resources to specific tasks and schedule the orders and times at which the tasks are carried out - to the convenience of the user of the system. The team has also devised resource management techniques for streaming data analytics, which can take in flows of information from sources including Twitter feeds and financial transactions. This was achieved through a variety of studies that Dr Majumdar has carried out in recent years.

In a 2017 study, Dr Majumdar and his colleagues developed techniques to effectively allocate and schedule tasks on cloud and cluster platforms by efficiently harnessing the resources of the systems. To gauge the effectiveness

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The diagram (based on [3]) shows the middleware-based unification of geographically dispersed resources, which can be shared by various users through a two-level communication system comprising local access networks that are connected to the main back-bone network.

of their techniques, the team paid attention to maximising the quality of service of the systems, based on the requirements of users. To do this, Dr Majumdar's team created an algorithm that effectively performed resource management on systems that processed open streams of batch data analytics jobs, in which the large data file was split into smaller chunks each of which was processed by a set of concurrent tasks in the job. For each task, the algorithm set an earliest acceptable start time, a required execution time, and specified which particular tasks should be started after another has finished. These times were ultimately derived based on what the user had specified as a deadline for completion through a service level agreement. After analysing the performance of the algorithm, Dr Majumdar's team found that compared to a leading previously developed technique, 63% fewer overall tasks missed their deadlines when using their algorithm.

In the same year, Dr Majumdar led a further study that explored how energy consumption could be reduced in cloud and cluster-based systems. Unsurprisingly, processing huge amounts of data requires systems to consume huge amounts of energy, accounting for a large fraction of their maintenance costs, and making significant contributions to greenhouse gas emissions. To address this pressing issue, Dr Majumdar's team developed their algorithm further to take the energy consumption required for each smaller task into account. This time, the algorithm could match tasks together to be performed at the same time, and adjust the CPU operating frequency in such a way that energy consumption was reduced while the quality of service requirements of users could still be met. After testing the updated algorithm in a range of scenarios, the team achieved a reduction in energy consumption of up to 45% for a simulated cloud system and workload – potentially a hugely significant step towards energy-efficient data centres.

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Again in 2017, Dr Majumdar and his colleagues started analysing how streaming data analytics that concerns extracting information from continual streams of data could be performed more efficiently. Particularly for social media companies such as Twitter, information needs to be processed and scheduled in particular orders, based on whether one piece of information has priority over another. Multiple levels of priority are often needed as well in the context of smart systems generating sensor data streams that need to be processed in real time. To address the issue, the team developed two scheduling techniques. These could assign higher priority to information to be scheduled depending on whether the system is 'static' (where the priorities are unlikely to change), or 'dynamic' (where priorities can continually change). After prototype implementation, the team demonstrated how their proposed scheduling techniques can be highly effective.

Platform for Managing Smart Systems

As well as working with processing platforms, Dr Majumdar and his team are dedicated to analysing unified systems of many computer systems, scattered over many geographical locations. This is often required in the management of sensor-based smart systems. Such systems leverage the 'Internet of Things' (IoT) technology for communication among a large number of independent objects, which are often found in sensor-based bridges, buildings, machinery and patient monitoring systems.

One problem currently facing IoT technology-based smart systems is the difficulty of basing the smart system component being monitored in one location while having the tools and computing systems required for the analysis of its data in other places. Through several recent studies, Dr Majumdar and his colleagues have created middleware to act as a 'glue' that connects various system components, allowing a variety of data sources and tools to become available on demand. The advances will allow authenticated users of smart systems to analyse data and manage devices from anywhere in the world.

In 2015/2016, a team led by Dr Majumdar described how a cloud-based system could be used to effectively manage large IoT-based smart systems. Despite these systems having widely varied management needs, all smart systems share the same basic operations: monitoring the state and health of their infrastructure and analysing and making decisions on their future states and maintenance. Smart systems require various different resources to carry out these tasks, including computers for data analysis, storage for sensor data and maintenance history, and software for analysing sensor data. Dr Majumdar's team realised that clouds can help to manage such complex smart systems by unifying dispersed resources required for managing a smart facility. In two case studies, they showed that cloud-based systems can greatly improve operation in smart systems of geographicallyscattered resources.



The figure (based on [1]) presents the architecture for a remote patient monitoring system. Wearable Health Sensors (WHS) send sensor readings to the mobile device, which uses the embedded Complex Event Processing (CEP) Engine to detect complex events and send them to the remote IoT Hospital Server (IHS) for further processing at the backend and notification.

Dr Majumdar and his colleagues also explored how cloud-based platforms could be used in research collaboration. In a 2015 study, the team proposed a system where privately-owned software and hardware resources are linked together into a unified platform, available for use by different groups of researchers working in the same field. Named the 'Research Platform for Smart Facilities Management' (RP-SMARF), the system would allow researchers to carry out tasks using resources and datasets that would have previously been unavailable to them.

Perhaps the main appeal of RP-SMARF is the ability of researchers to access data generated by experiments at any location around the world. Through a sophisticated authorisation framework, resource owners would be able to precisely control the availability of particular elements to other users of the system, allowing for a secure, trustworthy way of sharing information about experiments. Dr Majumdar's team believes that RP-SMARF will unify researchers around the world, significantly increasing their productivity. In addition to facilitating research collaboration, RP-SMARF-like systems could be used to monitor and manage smart facilities and extend

the lifespan of public infrastructure including buildings, machinery and renewable energy sources such as wind turbines and hydroelectric dams. The system would allow this by helping engineers to collaborate and share streams of data from the smart system with one another over many locations. With this greater ease of communication between engineers, the inspection, maintenance and repair processes of public infrastructures could be made far more efficient.

In their latest studies, Dr Majumdar and his team have introduced an architectural framework for performing complex event processing for smart systems. A complex event is a combination of multiple raw events, each of which may correspond to the respective sensor data crossing a predetermined threshold value. The team proposed a smartphone-based, remote patient monitoring system that uses data from sensors attached to patients' bodies to detect complex events that may indicate impending health problems. Currently, mobile devices that forward sensor data streams to hospital servers need to remain connected to the server and increase the consumption of the overall network when large amounts of data are transferred. However, the

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smartphone-based system can process complex events on the device itself and is therefore able to generate local alarms for the patient in the event that the mobile network becomes temporarily unavailable, disconnecting the user from the hospital server. The researchers demonstrated the viability of their approach through a proof-of-concept prototype built from a Google Pixel smartphone, and open source software. Analysis of the device's performance provided new insights into how patient monitoring systems can be scaled, and into the relationship between the complexity of the system and its performance.

The research performed by Dr Majumdar and his colleagues was carried out in the laboratories of the *Real Time and Distributed Systems* (RADS) Research Centre in Carleton University. With internationally recognised researchers and talented graduate students, the centre is a seat of world class research in real-time and distributed computing systems. Dr Majumdar and his team are currently engaged in further research in each of the two themes: resource management on big data processing platforms and platforms for managing smart systems.



Meet the researcher

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Dr Shikharesh Majumdar is internationally known for his research in resource management and middleware for high performance parallel and distributed systems. He is a Full Professor and the Director of the Real Time and Distributed Systems Research Centre at the Department of Systems and Computer Engineering in Carleton University, Ottawa. He was awarded his PhD in Computational Science from the University of Saskatchewan in 1988. Dr Majumdar's research interests are in the areas of cloud and grid computing, smart systems, operating systems and performance engineering. He has received a number of awards for his research and services to the professional community, including the IEEE's Best Paper Award in 2017, the Glory of India Award and Recognition of Service awards from ACM and IEEE. He is a member of ACM, is a senior member of IEEE and has provided lectures in various countries as a Distinguished Visitor for The IEEE Computer Society (1998-2001).

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CYBERFORENSIC.NET – TRAINING MANY TO FIGHT CYBER CRIME

People are sharing more personal information online than ever before. It is essential, therefore, that robust security and privacy systems are in place to protect it. Furthermore, experts in the field of cybersecurity are essential. Drawing on their extensive research experience in the field of internet security, **Dr Yier Jin** of the University of Florida and **Dr Cliff Zou** of the University of Central Florida have created cyberforensic.net. This website aims to enrich the cybersecurity workforce by providing training in the areas of digital forensics and internet security.

The Promise & Pitfalls of the IoT

The Internet-of-Things (IoT) has revolutionised the way we interact with society and the world. Briefly, the term 'Internet-of-Things' refers to the collecting and sharing of information between computers, electronic devices and humans by means of the internet. It may involve anything from mobile phones to jet engines. If it can transmit useful and beneficial information between device and user through the internet, it is part of the IoT.

The IoT is already having a huge impact on our lives. Most companies, government agencies and ordinary people rely on the cyber world for information and data management, processing and exchange. For example, many of us use our devices to pay bills and buy groceries. Many use devices to monitor the performance of systems remotely. And of course, most of us use the internet to communicate with others.

However, the dependence on IoT-based systems introduces challenges. Given the personal nature of the information exchanged by these means, maintaining security and privacy is of utmost importance. Consider, for example, online fraud – the act of deception over the internet for financial gain. According to estimates, some \$16.8 billion was stolen in 2017 by way of fraudulent activity. As a result, the call has gone out to greatly strengthen our cyber-defence systems to better respond to attacks.

Part of this involves skilling up individuals who, using their newfound expertise, can improve and implement enhanced digital security systems. To get the ball rolling on this, Dr Yier Jin of the University of Florida and Dr Cliff Zou of the University of Central Florida have created cyberforensic. net – a website that aims to enrich the cybersecurity workforce by providing training in the areas of digital forensics and IoT security.

During the website's creation, Dr Jin and Dr Zou were able to draw on their wealth of research and development experience in these fields. Examples of their previous contributions are discussed below.



A Fraud Detection Mechanism for Online Merchants

As the use of online marketplaces and digital transaction technologies becomes more customary, acts of fraud by these means are frighteningly common. There has never been a greater need, then, to protect every individual's financial data. This is especially true as many retailers move towards so-called 'Card Not Present', or 'CNP' schemes, where transactions can be made without presenting an actual credit or debit card at the time of purchase. 'The development of an online digital forensics program will reshape current cybersecurity education practices and improve related outcomes. It does this by providing a more comprehensive and thorough atmosphere in which students and professionals can study and build their expertise in the field cybersecurity, and ultimately, prevent cybercrime.'



While CNP offers several benefits for consumers, the absence of face-to-face contact means that merchants cannot positively ascertain the cardholder's identity. Moreover, merchant security systems themselves are far too simplistic and easy for hackers to bypass. They are often based on the merchant's own history of fraudulent activity, and so are not adaptable to emerging methods of fraud. Remember too, there is time lag between when a fraudulent transaction occurs and the time when it is reported by the cardholder.

To fight against this type of fraud, Dr Zou, Dr Jin and their colleagues developed an innovative fraud detection model that can be implemented by online merchants. Their model directly interacts with the buyer's electronic purchasing device (a computer or a smartphone) and combines it with a statistical concept known as a buyer's 'diversity index'. The technology essentially assesses a buyer's previous purchasing patterns and looks for anomalies that may indicate fraudulent activity. The team's proactive anti-fraud technique has proven to be incredibly effective. In the associated paper, they highlighted, 'our method has been tested against real transactional data and yielded exceptional results with the ability to detect even previously undetected fraudulent transactions.' Armed with this approach, online merchants may be able to significantly reduce instances of fraud.

How Attackers Can Get Around Traffic Shaping

Traffic shaping, or packet shaping, refers to the practice of regulating network data transfer speeds, to maintain certain levels of internet performance. Traffic shaping is often employed to control usage over free Wi-Fi connections, such as those offered by fast food restaurants, coffee shops, hotels, and airports. Limiting speeds prevents a single user from overloading the hotspot and pushing out others. However, hackers can bypass traffic shaping systems and essentially steal internet speed.

To investigate this practice, Dr Zou, Dr Jin and a colleague assumed the role of

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'attacker' – investigating the methods by which traffic shaping systems can be overcome. Their approach involved creating multiple wireless clients that emulate separate wireless devices. They then combined all of these into one physical wireless interface card. The result was an amalgamation of multiple connections and a significant increase in internet speed. The team concluded that a would-be attacker could achieve a 16-fold increase in internet speed using this technique.

The Cyber Attack & Defence Relationship

Cyberattacks are, in a sense, warfare – an interaction between attackers and defenders. And like warfare, the associated interactions are dynamic. However, in a research paper published in 2018, Dr Zou explained that current models of cyber-attack behaviour often do not recognise this fact: 'Most of the cybersecurity research focus[es] on either presenting a specific vulnerability or proposing a specific defence algorithm to defend against a welldefined attack scheme... Few have paid attention to the dynamic interactions



between attackers and defenders, where both sides are intelligent and will dynamically change their attack or defence strategies...'

Understanding that cyberwarfare is a dynamic process is vital when developing cyber defence algorithms and strategies. It offers deeper insight into attacker behaviour. So, the goal of Dr Zou's research was to design a cyberwarfare framework that considers this fact. In summary, their model was indeed able to better predict the progression of cyber-attacks and offered much more insight than typical fixed-strategy defence systems.

Training the Next Generation of Cyber-Crime Fighters

As the IoT continues to grow, and we share more personal information online, we will need a skilled up cybersecurity workforce. This in turn, creates a demand for effective training. With their invaluable experience in the field, that's exactly what Dr Jin and Dr Zou are working towards. 'The development of an online digital forensics program will reshape current cybersecurity education practices and improve related outcomes,' says Dr Jin. 'It does this by providing a more comprehensive and thorough atmosphere in which students and professionals can study and build their expertise in the field cybersecurity, and ultimately, prevent cybercrime.' And so, the duo launched cyberforensic.net in February of 2018.

Cyberforensic.net is a teaching and learning resource that imparts practical cybersecurity skills to students. There are several courses available. For example, it offers courses in incident response technologies, cyber operation and penetration testing, and malware and software vulnerability analysis. Each of these courses is supported with relevant lectures, notes and assignments. Another notable feature is the IoT and security related 'labs', or practical sessions. These have



been developed to expand digital forensic training beyond traditional personal computers to include emerging devices such as smart phones.

IoT training packages are also available to K-12 students. A series of so-called 'IoT Smart Car Labs' guides students through the basic principles of the IoT by way of hands-on, interactive activities. In the IoT Smart Car Lab 1, for example, the goal is to introduce young students to the IoT through a fun and interactive lab. 'A car will be constructed and equipped with motors and sensors,' says Dr Jin. 'The car can [be driven] over Wi-Fi from the student's laptop and the sensors can be read remotely as well.'

A Sharing of Cybersecurity Expertise

The cases discussed in this article are really just the tip of the cybersecurity iceberg, as it were. It is certainly an area that needs constant attention. Dr Zou and Dr Jin are developing an action plan to meet this challenge. Not only are they at the forefront of cyber-related trends and theory, they also aim to ensure that we have skilled individuals at our disposal to deal with cyber threats.

When asked about future aspirations, Dr Zou explained, 'the online digital forensics program will be offered to all graduate and undergraduate students majoring in computer science, computer engineering, and information technology at the University of Florida and the University of Central Florida.' And after a successful trial, they intend to expand the program by collaborating with other universities. 'The final goal,' Dr Zou relates, 'is to make the online digital forensics program available to all universities and community colleges nationwide.'





Meet the researchers

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Dr Yier Jin received his PhD in Electrical Engineering from Yale University, Connecticut, USA in 2012. After some time at the University of Central Florida, he became Associate Professor at the University of Florida's Department of Electrical Engineering and Computer Science, where he currently serves. His research interests include: The Internet of Things (IoT) and related security, Cyber-Physical System (CPS) design, resilient high-performance computing platforms, hardware-software co-design for system level security and protection, functional programming and proof writing for trusted IP cores, and trustworthy SoC architecture. He and his colleague, Dr Cliff Zou, have also created cyberforensic.net – an online cybersecurity training resource.

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