Australian Physics

VOLUME 60, NUMBER 1, JAN-MAR 2023

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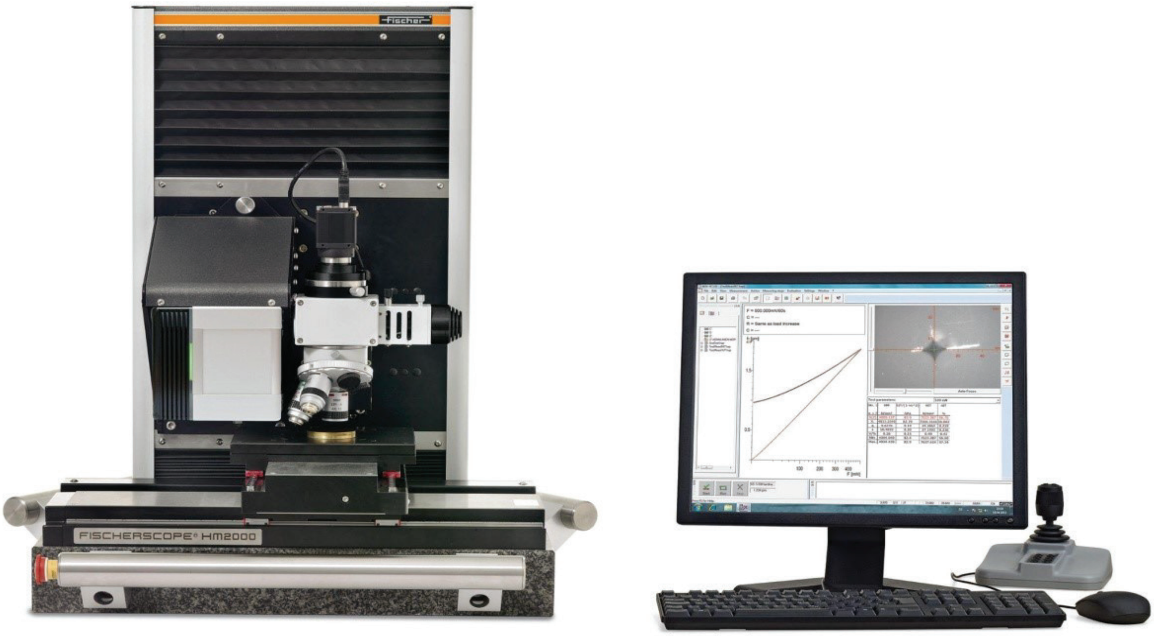

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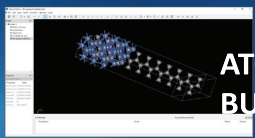

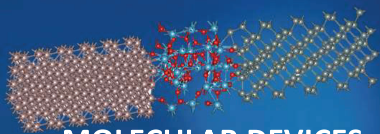

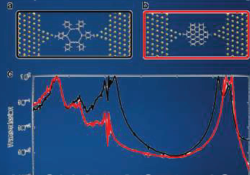

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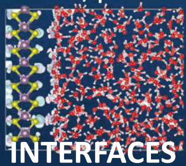

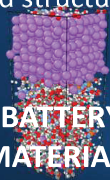

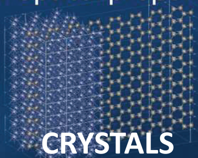

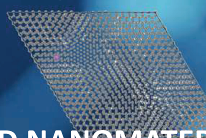

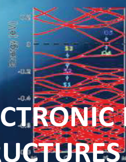

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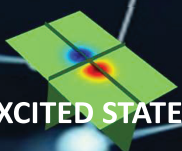

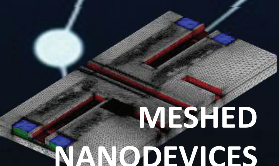

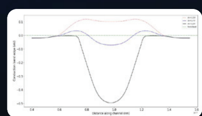

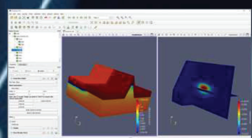

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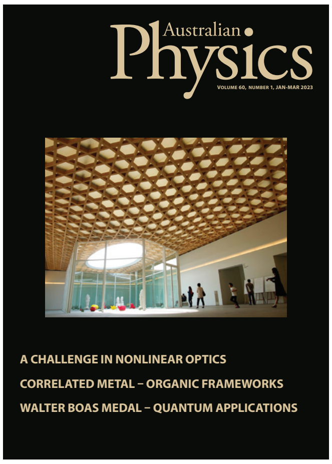

Architectural kagome lattice at the Oita Prefectural Art Museum, Japan. The gently curved structure could remind us of a flexible thin film or 2D material. Such materials with kagome crystal structure can exhibit unusual properties such as highly localised electronic states and magnetic moments. [credit: u\Gaijinloco; i.redd.it/48nib26tqex21.jpg]

Image on page 17: Basket in the style of traditional Japanese kagome weaving. [Adobe Stock]

Australian Physics

A Publication of the Australian Institute of Physics

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Articles or other items for submission to Australian Physics should be sent by email to the Editors. Only MS Word files will be accepted; a template with further guidelines is available online at the AIP websites (www.aip.org.au). The Editors reserve the right to edit articles based on space requirements and editorial content.

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Editorial

Sharing achievements

Quantum methods, 2D kagome materials, physics education, computation and data science, non-linear optics, and biophysics. Physicists add value to a plethora of fields, and the snapshot of areas covered in this issue of Australian Physics is only that – a snapshot. From developing an interest in physics, via studying physics, through to using the skills to build and foster a career, physicists in their generality have qualities that have to do with rising to challenges. This is not to diminish others; physicists do not hold a monopoly on meeting and overcoming challenges.

It is a good reminder, however, that solving challenges connects to achievements, and this issue of Australian Physics seeks to celebrate some of those achievements: important contributions to physics; distinguished careers; recent research in materials physics; and new 2022 AIP Fellows.

We also highlight how studying physics leads to careers in different fields and continents. As part of the broader innovation cycle in physics, we also spend some moments reflecting on physics education and the connection to delivering conferences in the field. Last but not least, we remember the life of Associate Professor Ian Desmond Johnston and his service to improving education through the use of innovation and technology.

Our next issue will be a special issue focusing on Australia's contribution to the field of Quantum Information Science and Technology. We are currently seeking contributions for the issue. Please get in touch at aip_editor@aip.org.au.

Best wishes,

David Hoxley, Clara Teniswood, Shermiyah Rienecker and Peter Kappen.

In Conversation with Nicole Bell

The Editors of Australian Physics sat down with Nicole Bell, the incoming AIP President. Nicole shares her thoughts on her journey in Physics, and the role of the AIP.

Tell us about your research interests

I'm a theoretical physicist at the University of Melbourne working on astroparticle physics – the intersection of the very small (elementary particles) with the very big (the Universe). The topics I've worked on have evolved with time. Earlier in my career, I worked heavily on neutrino physics. This was the main focus of my postdoctoral work at Fermilab and then at Caltech. In recent years, I've concentrated on dark matter physics, which led to my current role as leader of the Theory Program of the ARC Centre of Excellence for Dark Matter Particle Physics. Interestingly, there is increasing convergence of neutrinos and dark matter. For example, we will soon detect neutrinos in dark matter detectors (and, if we are lucky, perhaps vice-versa!) which is very exciting.

What is the role of the AIP?

I see the AIP as the voice for the Australian Physics community. Simply put, if someone needs wave the flag for physics in Australia, the AIP is the organisation that will do so. It has a key role in uniting the physics community across Australia, bringing people together for the Congress or Summer Meeting, state branch events, or outreach activities. The AIP has a particularly important role in promoting the value of physics to government and policy makers, and to the general public. In the last couple of years, AIP advocacy efforts have focused on physics education and research funding issues. We have sent letters and submissions to the Australian Research Council and government ministers, and had comments published in various media outlets. I am keen for this type of engagement to continue, with the AIP regularly playing a productive role in the national conversation on research and education.

What's your sense of the current AIP membership?

The current membership is heavily university dominated. In the last couple of years, the AIP has taken steps to develop better connections with industry. For example, we now have an industry advisory panel and we are looking at corporate membership options. We would like the AIP to represent all physics professionals in Australia, including those who work in academia, industry, defence, high schools, government organisations such as CSIRO or ANSTO, and beyond.

What do you want to do as president?

I think there is a need to advocate for the importance of supporting fundamental research. If you look at where national conversations about science funding are heading at the moment, there's a heavy focus on translation. And while that's important, we should take care to ensure that fundamental science does not fall off the agenda. Physics is a critical enabling science. History tells us that many technological developments were driven by fundamental research for which the eventual commercial applications were not originally anticipated. It is essential that basic breakthrough research is well supported, so that we feed the pipeline of ideas that ultimately lead to broad applications. We need a healthy balance of both.

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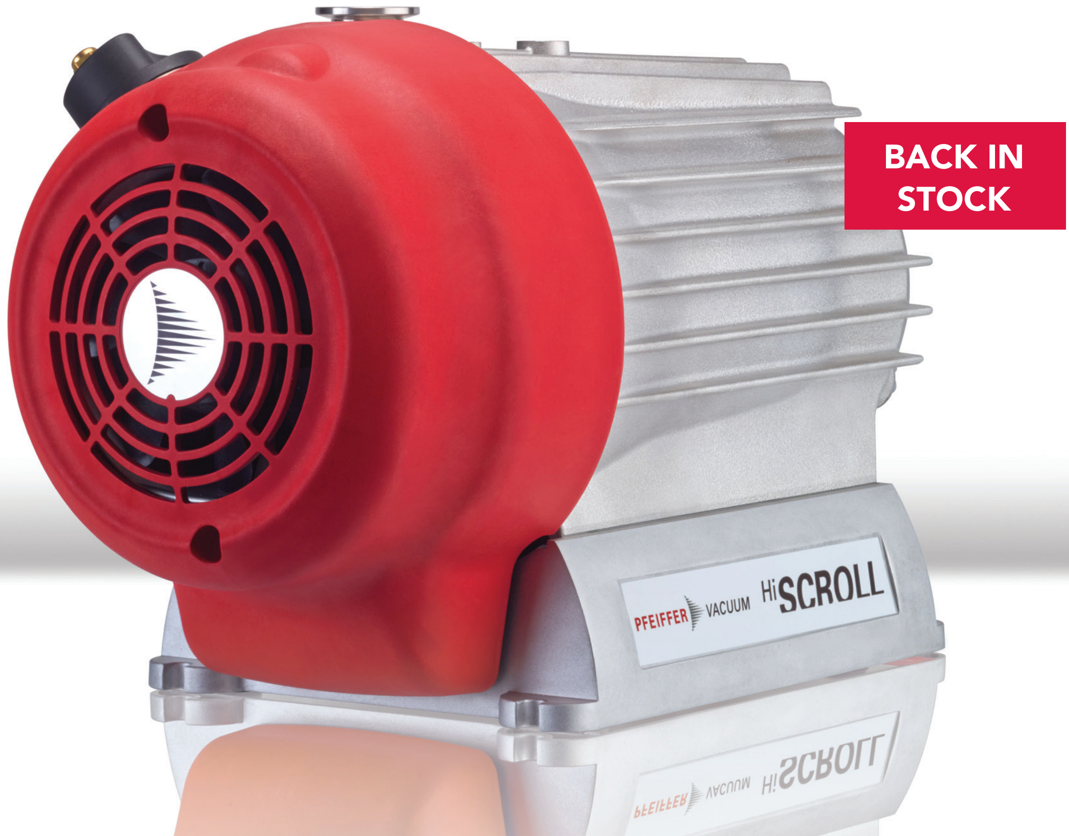

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Quantum applications and implications

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The Walter Boas medal is given annually by the AIP for the "research making the most important contribution to physics" done in Australia in the preceding four years. The citation for Howard Wiseman's award in 2021 is: "For elucidating fundamental limits arising from quantum theory, in particular in its applications to metrology and laser science, and via its implications for the foundations of reality." As this indicates, the work for which the medal was awarded was quite varied. In the article below, Professor Wiseman concentrates on two highlights: Heisenberg-limited lasers and a theorem stronger than Bell's.

Applications to metrology and lasers

Quantum theory implies fundamental limits to the performance of technologies, from measurement devices to computers. However, those limits are often far beyond what is achieved with 'standard' ways of building and operating such devices. When the fundamental limit (called the "Heisenberg limit" in some fields) scales better than the standard quantum limit (SQL), in terms of some basic resource – like time, size, or energy – we talk of a quantum advantage. This brings with it the potential for vastly better technology.

The best-known example of a Heisenberg limit is that offering a quantum advantage in the measurement of a static optical phase. Here, by using non-standard techniques such as entanglement or a variable number of beam passes, it is possible to estimate an initially unknown optical phase with mean-square error scaling as $1/N^2$. This is quadratically better than the SQL in terms of N, which represents the total number of photon-passes through the unknown phase shift.

I've worked in quantum phase metrology a lot over the years, in particular on the utility of adaptive measurements, and often in collaboration with experimentalists. This was reflected in some of my research in the Boas Medal period [1,2]. But, more excitingly (for me at least), in 2020, I and co-workers proved a Heisenberg limit of a completely new kind: for the coherence C of a laser beam in terms of μ, the mean number of excitations in the laser in steady-state [3]. Here C is also a dimensionless number: the number of photons emerging in the laser beam within one coherence time – in loose terms, the number of emitted photons with approximately the same phase.

The standard quantum limit to laser coherence is C scaling as μ^2, as proven by Schawlow and Townes in 1958 [4]. But, by reconceptualising the laser as any device that

a) Produces a beam close to that of a standard ideal laser beam,

b) Has no external sources of coherence,

we showed that a coherence scaling as μ^4, was possible [3]. For large μ, this implies a vastly greater coherence than a standard laser with the same μ. The key to achieving this is to make both the gain and output mechanism of the laser highly nonlinear processes, in a very specific way; see Fig. 1. Moreover, we proved a theorem that for any device satisfying (a) and (b), μ^4 is the best possible scaling [3]. That is, μ^4 is the Heisenberg limit to laser coherence.

In addition, we proposed a method by which this scaling could, in principle, be realised using superconducting quantum devices at microwave frequencies. That is, it would create a Heisenberg-limited *maser*, recapitulating the original technological development of lasers [4]. Subsequently, but independently, others had similar ideas [5]. Funded by a 2022 Discovery Project, with experimental partners in France, we are now working towards realising this type of device. As part of this DP, another PhD student with me at Griffith is currently working on a scheme to surpass the SQL scaling in an *optical* frequency laser.

Implications for the nature of reality

At the other end of the spectrum in quantum science are the field's implications for our understanding of nature. The most famous example of this is Bell's theorem from 1964 [6]. In this Bell showed that, if certain quantum experiments were to work as expected, then the conjunction of a certain set of metaphysical

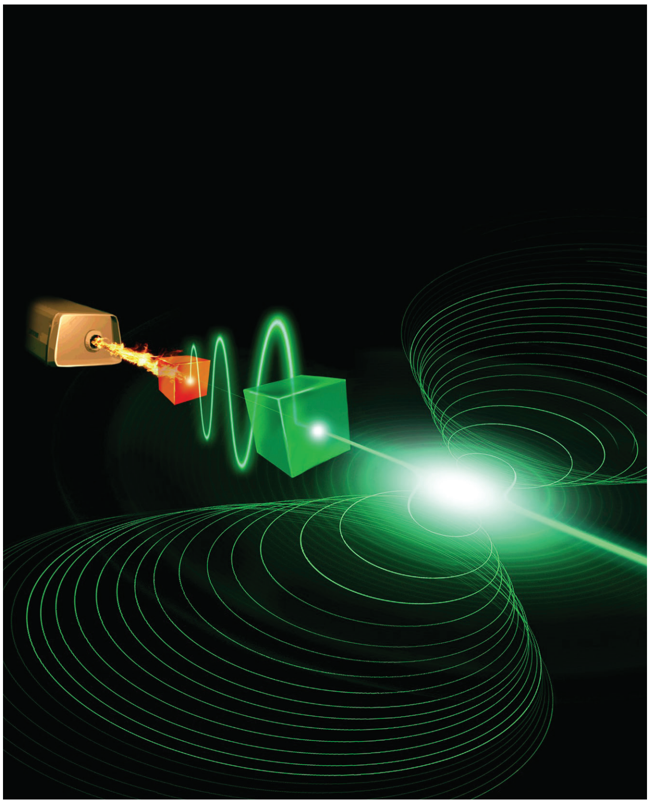

Figure 1: Artist's impression of a Heisenberg-limited laser, creating a highly coherent output from an incoherent input, by using non-standard gain and output processes. Credit: Ludmila Odintsova.

propositions – that is, basic statements about the nature of reality independent of any particular physical theory like quantum theory – must be false. Since 2015, when the first loophole-free Bell experiments were performed, we have been able to say that this set, in conjunction, *is* false. It was for one of these 2015 experiments, using entangled photon pairs, and its forerunners dating back to 1973, that the 2022 Nobel Prize in physics was awarded, to Clauser, Aspect, and Zeilinger.

There are many ways to choose the set of metaphysical assumptions that, in conjunction, Bell experiments rule out. Different authors go with different degrees of rigour and generality. For the purpose of this article, a convenient choice – quite general, and fairly rigorously stated – is the following:

(a) **Interventionist Causation.** If experimental interventions are made in a manner appropriate for randomized trials, then the only experimentally relevant variables that are correlated with the interventions are those of which the intervention is a cause.

(b) **Relativistic Causal Arrow.** Any cause of an event is in its past light-cone.

(c) **Absoluteness of Outcomes.** The outcome of a measurement is an *absolutely* real event, not relative to any-one/thing/world/branch.

d) **Causal Explanation.** If two variables are correlated then either one is a cause of the other or they have a common cause that *statistically explains* the correlation (in the sense that conditioning on the value of the common cause removes the correlation).

Note that the word 'cause' here does not have to be defined; its appearance in multiple propositions here is sufficient for the set, in conjunction, to imply the restrictions ("Bell inequalities") on correlations that have been violated experimentally. Note also that while (a) looks complicated, it is just a rigorous version of a sort of "free choice" proposition.

Now that loophole-free Bell experiments have been performed – proving that at least one of the four propositions, (a), (b), (c), or (d), must be false – what's next? As a warm-up answer, one future direction for Bell experiments is to replace proposition (c) by a *weaker* one, in which the property of absoluteness is required only for certain kinds of outcomes – the ones that we ultimately care most about [7]:

c') **Absoluteness of Observations.** An observation by a human being (or equally intelligent party) which can be communicated is an *absolutely* real event, not relative to any-one/thing/world/branch.

With this substitution, we can no longer say that the set (a,b,c',d) of propositions has been proven false experimentally, because intelligent parties are much slower at making observations than physical detectors are at producing outcomes. Thus (c') would require distributing entanglement to intelligent parties at much larger separations than has currently been achieved. However, such experiments, with one party on the moon for example, are certainly plausible in the medium-term [7].

Would such an experiment be worth doing? For most physicists, perhaps not. That is because, of either set (a,b,c,d) or set (a,b,c',d), most physicists already advocate giving up proposition (d). The reason is that standard quantum theory violates this proposition. In standard quantum theory, there are no common causes ("hidden variables" as they are often called) that statistically explain the correlations between space-like-separated measurements on entangled particles. And most physicists implicitly subscribe to a sort of scientific realism, in which the truth of a metaphysical proposition conforms to the truth of the corresponding

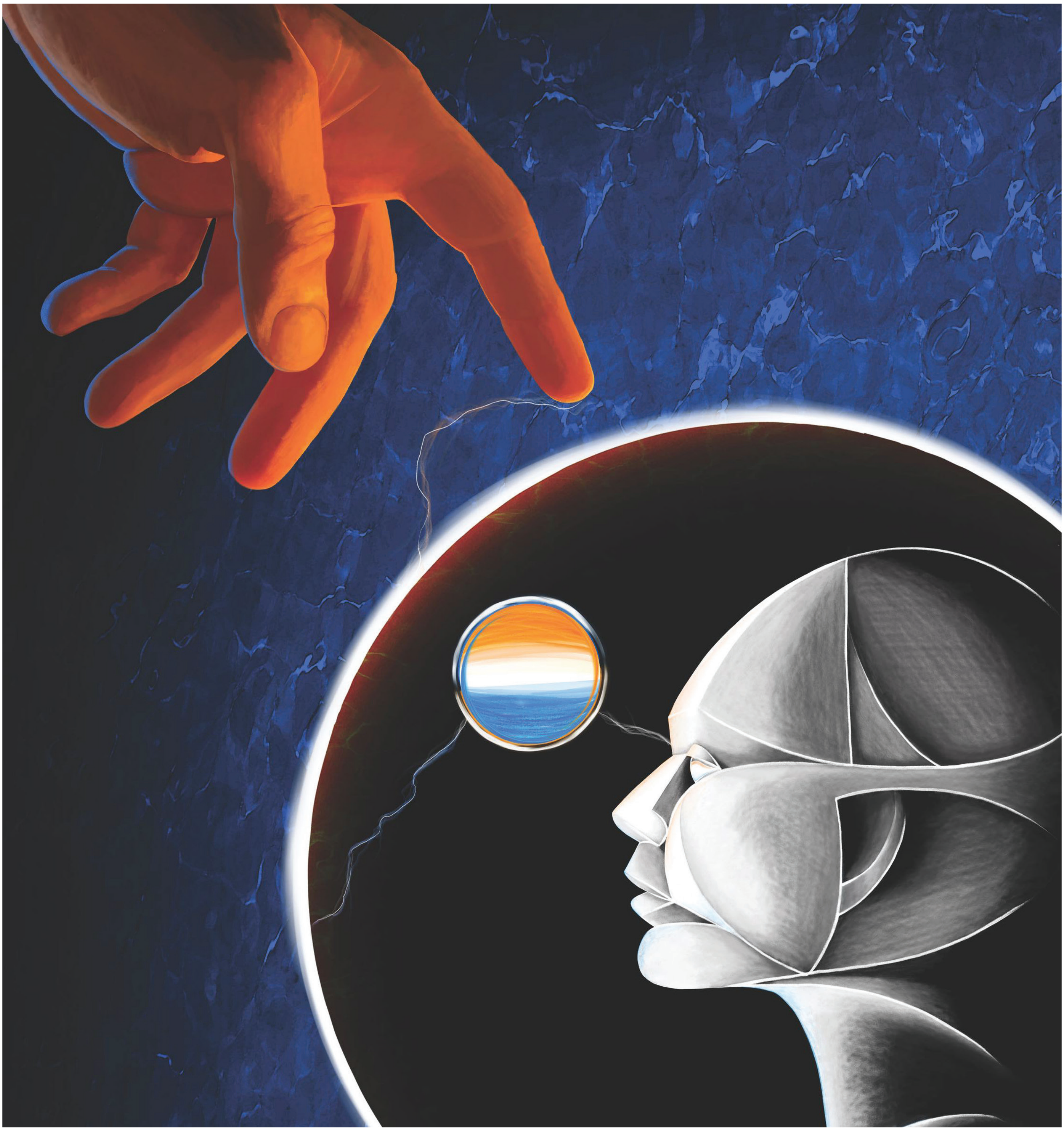

Figure 2: Artist's impression of a quantum computer instantiating an intelligent party who has observed a quantum system, perhaps about to be reversed at the whim of a human party. Credit: Tony Dunnigan.

proposition applied to our standard empirical description of physics (or other sciences).

Thus, I and my theory co-workers were shocked when, inspired by [8], we found a way to prove a theorem like Bell's but *without* using proposition (d) above, or anything like it. Specifically, in our 2020 paper [9], we proposed an experiment that, if it were to work as expected (by most physicists), would falsify the conjunction of just propositions (a,b,c) together. That is, our theorem is strictly stronger than Bell's theorem. The "easy way out", of rejecting hidden variables, no longer works. There is no proposition that "standard quantum theory" clearly rejects. Reality is constrained to be even stranger than Bell's theorem taught us.

The key to the thought-experiment in our theorem is the ability to reverse a measurement. Our co-workers at Griffith performed an actual experiment doing this, and saw violations of the new inequalities we derived

[9]. But we called this only a "microscopic proof-of-principle experiment", because there is no generally agreed criterion for a physical process or system to constitute a measurement or outcome, and, I suspect, most physicists would find the simple processes and tiny systems we employed unconvincing.

This is where proposition (c') comes in again. It gives a relatively unambiguous criterion for an outcome (here, elevated to an 'observation') to be absolutely real. Thus, ruling out (a,b,c') is, in my view, the most convincing way to rule out (a,b,c). But an experiment disproving the conjunction (a,b,c') would require technology far beyond that of today. As set out in detail in [10], it would need human-level artificial intelligence, and universal quantum computing at staggeringly large scale and speed. This would enable an intelligent party to observe half of an entangled pair of particles, thereby becoming entangled with a distant particle, while being run on a quantum computer that can be reversed, undoing the observation. See Fig. 2.

The experiment we envisage in [10] is much more difficult than the Heisenberg-limited laser experiment mentioned in the first half above. I do not expect it to be achieved in my lifetime, as it will likely take many decades of technological advancement. But I hope that our theorem is sufficient motivation for future generations of experimentalists to attempt that goal.

There is, I think, a small, but by no means negligible, possibility that an experiment with an artificially intelligent quantum computer would not give the results expected from standard quantum mechanics. If we, the scientific community, are lucky enough that this possibility is an actuality, then at some stage on the path towards that ultimate experiment we may well see deviations from expected behaviour. This, I hope, will motivate the current generation of experimentalists to begin the challenging trek along that path.

Acknowledgements

The recent work described here was supported by the Australian Research Council through Discovery Project grants DP170101734 and DP220101602, and the Centre of Excellence grant CE170100012 (Centre for Quantum Computation and Communication Technology), and by the grant FQXi-RFP-CPW-2019 from the Foundational Questions Institute and Fetzer Franklin Fund. I am grateful to my collaborator, Eric Cavalcanti, for feedback on the "Implications" section of this article. Finally, I would like to thank my PhD supervisor and long-time mentor, Gerard Milburn, for nominating me for the Boas Medal, and all my co-workers on the research for which it was awarded.

About the author

Howard Wiseman is an Australian theoretical quantum physicist. He is best known for his work in quantum control (manipulating matter and information at the quantum scale) and quantum foundations (trying to understand what is really going on when we do this). He is less known for his work in Arthurian history and literature. Howard has won several medals and prizes in Australia, but only for his physics research. He has been elected a Fellow of the Australian Academy of Science, the American Physical Society, and the Optical Society of America (Optica). He has been Director of the Centre for Quantum Dynamics at Griffith University since 2007.

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The mystery of a correlated metal-organic framework and how substrates change it

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Strong electron-electron interactions in materials give rise to effects such as magnetism and superconductivity. These effects have applications in magnetic memory, spintronics, and quantum computing. An emerging class of materials which can host strong interactions are two-dimensional metal-organic frameworks (MOFs). Two recent studies by Monash University have discovered one such MOF and illustrated how different substrates radically alter its electronic properties. The team showed how charge transfer, strain, and hybridisation influence electronic interactions as seen in the MOF's magnetic moments. Electric fields and applied strain could switch these interacting phases on and off, allowing potential applications in future energy-efficient electronics.

Introduction

With the ever-growing demand for digital technologies and the pressures facing conventional semiconductor electronics [1], there is a need for new nanoscale materials with new electronic properties. Strongly correlated materials – where electron-electron interactions cause different electron wavefunctions to become correlated – provide a potential solution, because such quantum interactions give rise to superconductivity, Mott metal-insulator transitions, quantum spin liquids, the Kondo effect, and magnetism.

Magnetism is a simple indicator of strong interactions, since it involves strong electronic repulsion preventing electrons of opposite spins from pairing.

One nanoscale structure with promise for correlated materials is the kagome lattice: a periodic array of corner-sharing triangles (Figure 1). Electrons in this lattice experience frustration due to the triangular motif. This can produce frustrated antiferromagnetism and quantum spin liquids, which have potential uses in quantum technologies. The frustration also produces destructive interference, localising electrons and enhancing electronic interactions. This makes the kagome lattice a prime system for exploring correlated phases.

While inorganic materials can have kagome lattices, a class of materials of growing interest are two-dimensional metal-organic frameworks.

Metal-organic frameworks (MOFs) are crystalline materials where organic molecules are connected by metal atoms. They have potential for low-cost synthesis in flexible devices. And MOFs can show many different properties by changing the molecules or metal atoms.

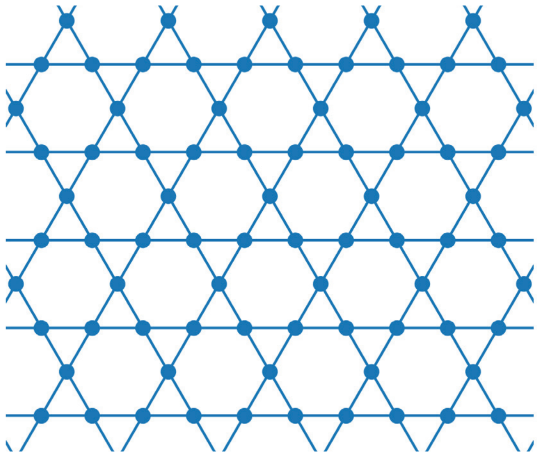

Figure 1: The kagome lattice. Atoms are arranged in a periodic array of corner-sharing triangles in a star-like arrangement.

As such, MOFs can be used to explore many different physical phases and a broad range of parameters. This includes correlated phases (e.g. [2]), although the exploration of correlated MOFs is still in early days.

Two-dimensional MOFs are often grown on solid, metallic substrates, which provide structural support and can provide a reactive surface necessary for growth. Electrical devices also require the 2D material to be connected to metallic leads. In 2D materials, the entire material forms an interface with the substrate, thus enhancing any effects of the substrate on the 2D material itself.

The mystery of dicyanoanthracene-copper

An intriguing example of a correlated 2D MOF is 9,10-dicyanoanthracene copper (DCA-Cu), which presents with DCA molecules in a kagome arrangement joined by copper atoms. Overlapping pi orbitals on the molecules allow electrons to hop between molecules. DCA-Cu can be synthesised on a Cu(111) surface by depositing DCA molecules in vacuum [3] and can be made on other substrates by also depositing copper atoms.

In recent experiments at Monash University, Kumar *et al.* grew DCA-Cu on an Ag(111) surface (Figure 2) [5]. Initially, this was intended as practice before synthesising DCA-Cu on an insulating substrate. Scanning tunnelling spectroscopy (STS) measurements detected a peculiar signature: a strong peak in the spectrum at zero bias voltage. This peak followed the spatial profile of the low-energy molecular orbitals (Figure 2a), indicating it was a feature of the low-energy electronic structure, and had a Fano lineshape (Figure 2c). The most distinctive signature for its cause was the temperature dependence, indicating a non-linear increase of the width with temperature (Figure 2d). These signs all pointed towards the Kondo effect as the cause of this zero-bias peak.

The Kondo effect is a many-body effect which arises due to coupling between a local magnetic moment (such as in a magnetic atom) and a metallic substrate. However, for DCA-Cu, this raised an important question: where did these local magnetic moments come from? Theoretical calculations and X-ray absorption spectroscopy [5] showed that the copper atoms of DCA-Cu were in a non-magnetic electronic configuration. The presence of magnetism in DCA-Cu required further investigation

Calculations find local magnetic moments

This question was theoretically investigated [5] using first principles (*ab initio*) density functional theory (DFT), which calculates the electronic properties just from the positions of atoms. While unable to simulate true many-body effects like the Kondo effect, DFT is capable of simulating magnetism, which is an essential prerequisite to the Kondo effect. The calculations found magnetic moments localised to the DCA molecules in the pattern of the low-energy molecular orbitals in a frustrated antiferromagnetic configuration (Figure 3). These magnetic moments had a fractional magnitude, suggesting a cause beyond simple electron counting arguments. To understand why magnetic moments appeared in the DCA molecules, the Hubbard model was considered. This is a minimal model of interacting electrons in a lattice with the Hamiltonian:

$$\hat{H} = -t\sum_{\langle i,j\rangle} \hat{c}_i^\dagger \hat{c}_j + U\sum_i \hat{n}_{i,\uparrow}\hat{n}_{i,\downarrow}.$$

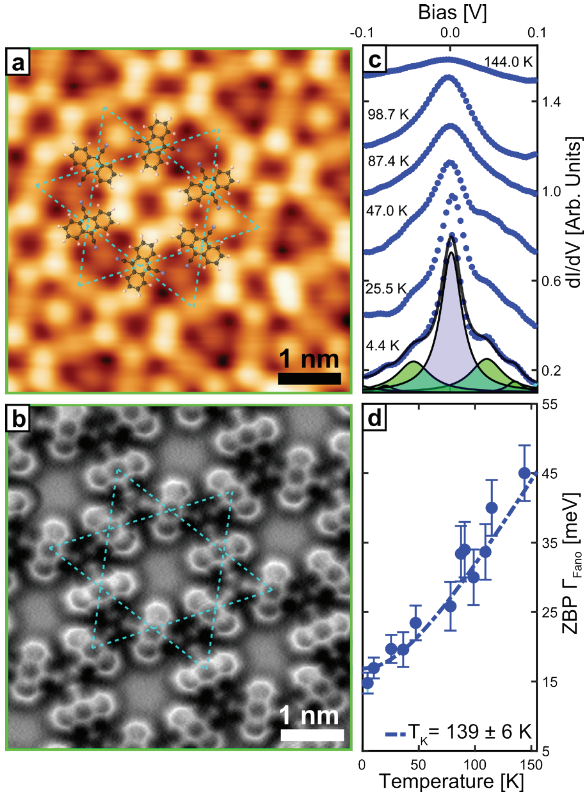

Figure 2. (a) Scanning tunnelling microscopy (b) and non-contact atomic force microscopy images of DCA-Cu on Ag(111). Note the kagome arrangement of DCA molecules (schematic superimposed). (c) Scanning tunnelling spectroscopy of DCA-Cu on the lobes of the DCA molecules at different temperatures. A fit of the zero bias peak is shown, along with satellite peaks associated with vibrational modes. (d) Width of the zero bias peak in (c) with respect to temperature. A fit to the Kondo temperature TK is included. Adapted with permission from [5].

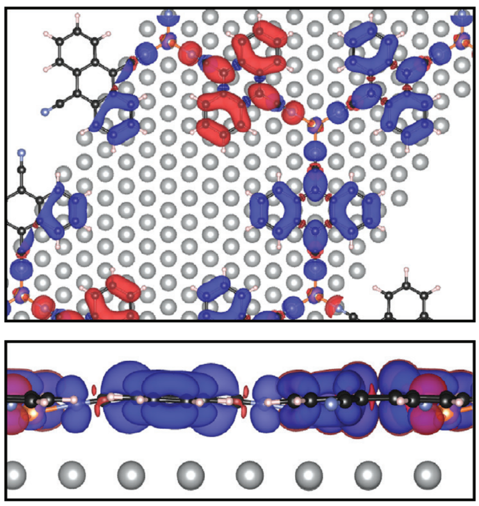

Figure 3. Magnetisation density of DCA-Cu on Ag(111), calculated by DFT. Top and side views are shown. Red and blue isosurfaces indicate opposite spin directions. Note how the magnetic moments are localised to the molecular orbitals of DCA. Reproduced with permission from [5].

The first term describes electrons hopping between adjacent lattice sites with amplitude t. The second term describes electrons of opposite spin on the same site repelling each other with strength U. To solve this model, the Hartree-Fock approximation was used, which considers only interactions with the average electron density. Similar to DFT, the Hartree-Fock approximation is capable of simulating magnetic phases.

Each DCA molecule was modelled as a single site in the Hubbard model. Despite the great simplicity of this model, the calculations [5] found excellent agreement between the Hubbard model and DFT results. This indicates that the magnetism was caused by strong interactions within the DCA molecules of the MOF, as described by the Hubbard model. This showed that DCA-Cu was a MOF with strong electronic interactions between electrons hopping about the kagome lattice.

This work [5] used the Kondo effect as a probe of local magnetic moments and strong correlations. It showed that DCA-Cu is a strongly correlated 2D MOF.

Different substrates, different behaviours

However, these experiments raised further questions. While the Kondo effect and magnetic moments were observed for DCA-Cu on Ag(111), they were not observed on Cu(111). Copper and silver are both noble metals. So why did the MOF behave so differently on different substrates?

The team performed further DFT calculations [6] with different substrates to determine under what conditions magnetism could emerge. The chosen substrates – Ag(111), Cu(111), Au(111), Al(111), graphite, and hexagonal boron nitride (hBN) on Cu(111) – represented a range of work functions and reactivities and included several experimentally relevant systems.

The Hubbard model was also extended to include coupling to a substrate. This model accurately described many of the physical phenomena in the atomistic simulations and allowed for a exploring a wider range of systems quickly and easily with fine control over the important parameters. The fine-grained parameter sweeps of the Hubbard model corroborated the general trends suggested by the DFT calculations of the chosen substrates.Three key variables were found to determine the effect of substrates on electronic interactions: charge: transfer, strain, and substrate hybridisation.

Charge transfer occurs when a substrate gives or takes electrons from the 2D material. This is influenced by the relative work functions of the MOF and substrate. Magnetism was strongest when the material had one free electron per molecule (i.e., half-filling) because this allowed a full unpaired spin on each molecule. This is shown in the horizontal axis of the phase diagram in Figure 4.

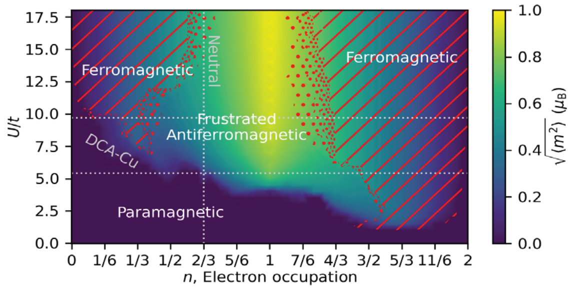

Figure 4. Magnetic phase diagram of the kagome Hubbard model (without a substrate), indicating the strength of the local magnetic moment $\sqrt{\langle m^2 \rangle}$ Calculated by the Hartree-Fock approximation. Transition phases between antiferromagnetic and ferromagnetic are marked with red dots. The values of *U/t* corresponding to DCA-Cu are marked, as is the electron occupation for neutral DCA-Cu. Note how the magnetism is enhanced towards half-filling and larger *U/t*. Adapted from [6].

Strain happens when a substrate stretches or squeezes the 2D material. When the material is stretched, the overlap between adjacent molecular orbitals is reduced, which reduces the hopping (t) of electrons between molecules. This localises electrons, making them experience local interactions more strongly (i.e., it increases U/t). This is shown in the vertical axis of Figure 4.

Hybridisation occurs when the electronic character of the substrate and the 2D material are mixed due to coupling between them. Metallic substrates often show strong hybridisation, which can suppress magnetism. But insulating substrates, such as atomically thin hBN, exhibit very weak hybridisation and preserve the intrinsic electronic interactions in the material.

These three variables explained the trends observed between the substrates. Charge transfer was a major predictor, with electron occupations near half-filling providing much stronger magnetic moments and greater robustness against substrate hybridisation. Hybridisation, when present, could greatly weaken the magnetic moments. And strain adjusted the magnetic moments further, sometimes tipping the balance between magnetic and non-magnetic. Knowing these trends allows us to understand why different substrates behave differently.

Tuneable control over emergent magnetism

With this understanding of the key variables, it is possible to consider how to manipulate these variables to control the electronic interactions. One could hypothesise that certain external stimuli would move the systems to different parts of phase space, switching the magnetic phases. These hypotheses were tested by further DFT calculations [6].

An electric field could turn magnetism on and off by changing the charge transfer. Moving charge into DCA-Cu when on Cu(111) allowed magnetism to emerge where before there was none. Moving charge out of DCA-Cu when on hBN on Cu(111) turned off the magnetism where before there were very strong magnetic moments. Having electric control of magnetic phases is vital for using these materials in electronic devices.

Applied strain could also turn magnetism on and off. DCA-Cu on graphite naturally received compressive strain from the substrate, reducing the magnetic moments. However, applying tensile strain to DCA-Cu on graphite enhanced the magnetic moments. and Going forward, strain is also an important consideration for flexible electronics.

Understanding which variables control correlations in these materials enables rationally choosing external controls to alter the correlated phases. This is a vital step towards designing practical devices from these materials.

Conclusions and future directions

These studies have identified strong correlations and local magnetic moments in a 2D kagome MOF, revealed by experimental measurements of the Kondo effect and by DFT calculations and modelled by the Hubbard model. The work also showed how choice of substrate changes correlations within 2D materials through charge transfer, strain, and hybridisation (Figure 5). These predictions, made for a wide range of substrates and conditions, can guide future experiments on these systems.

2D MOFs provide a rich platform to explore novel quantum physics applied for energy-efficient electronic devices. While the DFT calculations focused on the case study of DCA-Cu, the Hubbard model is generalisable to any kagome material. These findings suggest that there may be other correlated MOFs out there, just waiting for the right substrates or conditions to reveal their special properties. We hope these works aid in the rational design of novel electronic devices and in the on-going quest to understand strongly correlated materials.

We are currently investigating more advanced methods for simulating strong interactions between electrons. These methods will allow for directly simulating the Kondo effect, along with other technologically relevant effects such as Mott metal-insulator transitions. The team at Monash is also experimentally investigating DCA-Cu grown on some of the substrates considered theoretically, where we hope to find further evidence of strong correlations.

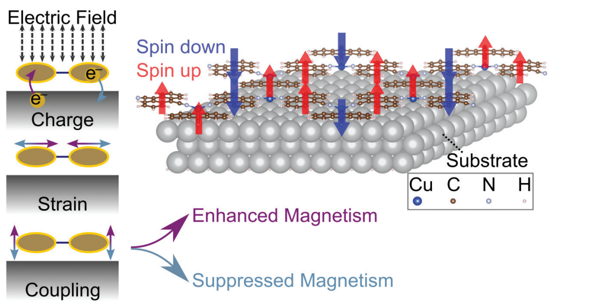

Figure 5. We found local magnetic moments in a 2D kagome MOF on substrates. Charge transfer towards half-filling, tensile strain, and weaker substrate coupling enhanced the magnetism, while the opposite suppressed the magnetism.

About the author

Dr Bernard Field recently completed his PhD at Monash University with the ARC Centre of Excellence in Future Low-Energy Electronics Technologies (FLEET) and has recently taken up a post-doctoral role at Berkeley, CA. His research focuses on exploring the quantum properties of materials by computational and theoretical means. He enjoys collaborating with his experimental colleagues to discover new questions to research.

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IUPAP International Conference on Physics Education 2022

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The IUPAP has Commissions which focus on different aspects of physics. Commission C14 focuses on Physics Education. The flagship conference of C14 is the International Conference on Physics Education, ICPE. It was hosted by Australia for the first time in December 2022. This was a unique opportunity to showcase physics education in Australia to the world. Here we will describe the conference, discuss the benefits and disadvantages of online conferences over face-to-face conferences, describe the variety of conferences available in the field of physics education and discuss trends in physics education as observed from themes arising from the conference. We have documented how we planned and ran this conference, and it is available online at icpe2022physicseducation.com/lessons-learnt-and-advice/. We hope this is useful for others planning online conferences in the future.

The International Conference on Physics Education (ICPE) 2022 was hosted by Australia with co-hosts in Thailand and Indonesia from 5th-9th December 2022. The conference was held online with 268 registrants from 43 different countries. 106 of these registrations were from Australia. The theme of the conference was "Physics Education: Preparing for the Future". Participants included academics teaching undergraduate physics, academics teaching future high school teachers as well as high school teachers. Our aim was to make the conference accessible to all. We achieved this through offering many fee-waiver scholarships, minimising costs and accounting for different time zones and busy schedules.

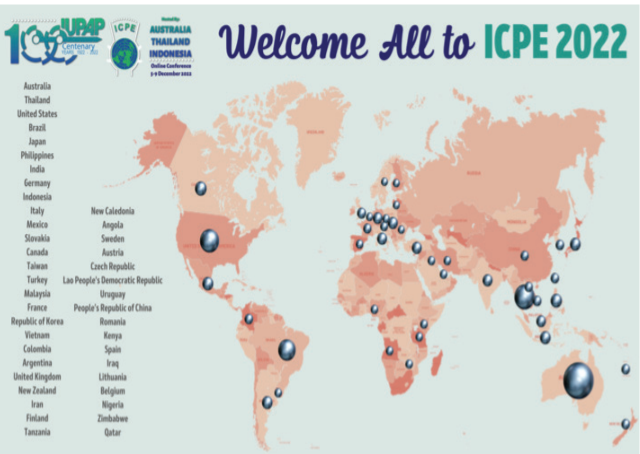


Figure 1: Countries represented by participants at the conference.

History of ICPE

The International Commission on Physics Education was conceptualised by a group of physicists in the late 1950s. A request submitted to IUPAP for an education related commission was granted before the end of the year. The Commission on Physics Education is officially Commission C14: Physics Education, established in 1960 under the umbrella of IUPAP. It promotes the exchange of information and views among the members of the international scientific community in Physics Education, for example by organizing and endorsing conferences, publishing a Newsletter and producing Handbooks. C14 also awards the ICPE Medal to those who have made significant enduring contributions and whose influence is international. The aim is to improve the teaching of physics worldwide, mainly in the 60 countries associated to IUPAP. Manjula Sharma is currently the Vice Chair of Commission C14 and is also Editor of the ICPE Newsletter.

The International Conference on Physics Education, (ICPE) is the flagship conference of Commission C14 of IUPAP. The first ICPE occurred in 1960 in Paris, followed by Rio de Janeiro in 1963 and London in 1965. The aim is to run ICPE every year, and it mostly does. Often it partners with other conferences such as the International Research Group on Physics Teaching (GIREP) or the World Conference on Physics Education (WCPE). 2022 was the first time ICPE has run from Australia. ICPE 2023 will be run from Punjab, India.

Education conferences

There are numerous educational conferences available to people in Australia, each filling its own niche. Here we will describe the recurring ones, who they are aimed at and when they will run next. Information on the latest conferences can be found in the AIP Physics Education Group (PEG) newsletter. Email the authors if you would like to subscribe to this list or select PEG as a topical group when you register with the AIP.

The **AIP Congress** and **AIP summer meetings** are held in December in alternate years. These are face-to-face whenever possible. The PEG is active at these conferences, hosting talk sessions and workshops. These sessions are generally aimed at academics teaching physics to undergraduate students; the aim is to ensure the sessions are suitable for people with different levels of exposure to educational research. The PEG AGM is held at the AIP Congress in years it runs. The AIP summer meeting will be held in Canberra this year, and then the AIP congress will be held in Melbourne in 2024. This is an excellent opportunity to network with other academics teaching physics.

The **Australian Conference on Science and Mathematics Education** (ACSME) is held each year at a different Australian university. This conference is usually aimed at academics teaching across the science disciplines. The conference runs over two days with the third day being a "discipline day". PEG runs a workshop and holds our AGM at ACSME on years the AIP congress does not run. This is a great conference to attend if you are interested in getting into physics education research. In 2023 this conference will be held at the University of Tasmania from 30th August – 1st September.

CONASTA is the annual **Conference of the Australian Science Teachers Association**. It is aimed at high school science teachers, school laboratory technicians and people working in high school science education. In 2023 CONASTA 70 will be hosted by the South Australian Science Teachers Association (SASTA) between 9-12 July. Most of the states also hold their own science teacher conferences throughout the year. Many of these have a physics stream.

Besides ICPE, the main international annual conferences are the **American Association of Physics Teachers (AAPT) conferences** that happen twice a year, with a summer and a winter meeting, the summer meeting being the larger. The next of these is held in Sacramento, California from July 15-19. This is a really great opportunity to hear about educational research across the USA and to see some novel teaching practices. **GIREP** is the annual conference of the International Research Group on Physics Teaching, the Physics Education Division of European Physical Society. It is similar to the other international conferences but Europe-focussed. The next conference will be held 3-7 July 2022 in Košice, Slovakia.

Online, face-to-face or hybrid?

Since the COVID-19 pandemic we have all had many experiences with online conferences. When we were considering whether to host our conference online, face-to-face, or hybrid, our main considerations were twofold. Firstly, we wanted the conference to be affordable to everyone. We were very aware of the travel and accommodation costs to Australia for people in other countries and were keen to avoid these. Expensive conferences mean that people from many countries in the world, and most school teachers, cannot participate. Secondly, we were worried about the uncertainty around travel with borders opening and closing. Making the decision to make the conference online from the start gave us certainty and allowed us to plan for the best possible online experience for everyone.

There are advantages and disadvantages to both online and face-to-face conferences. The big advantages of face-to-face over online conferences are that it is easier to network and meet new people (conversations happen more naturally), and that most people in attendance have taken time off work and are away from personal and family demands and so are able to engage in social activities at the conference.

There are several big advantages of online conferences, too. They are cheaper to run so there is no need to book venues, as well as cheaper for participants as no accommodation or transport. If talks are recorded, people can watch multiple talks that are on at the same time. They are also better for the environment; you do not have the greenhouse gas emission associated with all the flights that a face-to-face conference entails.

A disadvantage of online conferences is that people are in different time zones. While this means that people do not need to deal with jet lag it does mean people are either attending events in the middle of the night or talks need to be recorded and made accessible which decreases the level of interaction.

Hybrid conferences can have some of the advantages and many of the disadvantages of both online and face-to-face but it can be challenging getting online participants to interact with those face-to-face. It can be similar to running two separate conferences and so twice as much work for the organisers.

Ultimately, which format will be most suitable depends on the aim of your conference.

Running online conferences

You can view our conference website at icpe2022physicseducation.com. Good educators apply reflective practice, looking back at what they have done to improve for the future. While we have no immediate plans to run another conference, we thought there could be benefit to others in documenting how we went about it and what we would do differently if we were running this again. We have documented all this at icpe2022physicseducation.com/lessons-learnt-and-advice/ along with template files that you may find helpful if you are planning an online conference. These include instructions we put together for casuals on how to run the zoom rooms, workshops, online forms we used to collect information from participants and templates for communications.

Our top tips for running an online conference are as follows.

Communicate clearly and regularly with participants. We sent out daily emails with a timetable and zoom links so that participants did not have any trouble knowing what was on each day or how to access it. These emails were mail-merged, so we assigned each participant a unique "zoom name", a number followed by their name, in order to keep track of attendance.

Use a **"Virtual Poster Platform" for posters** as well as to **provide links to the recordings** of each of the sessions. People had access to the talks at the end of each day. This worked exceptionally well. The link was only provided to people who had registered.

Use the social media app discord to **communicate among the technical committee in the lead up to the conference and with the casuals assisting with the conference**. This was incredibly useful, we felt very connected and were able to quickly fix problems despite working in different locations.

Train technical staff well. We had a practice dry run for the different session types, and have run sheets for

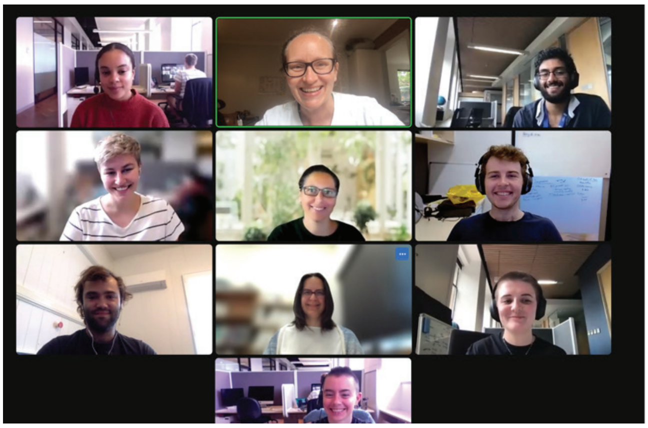
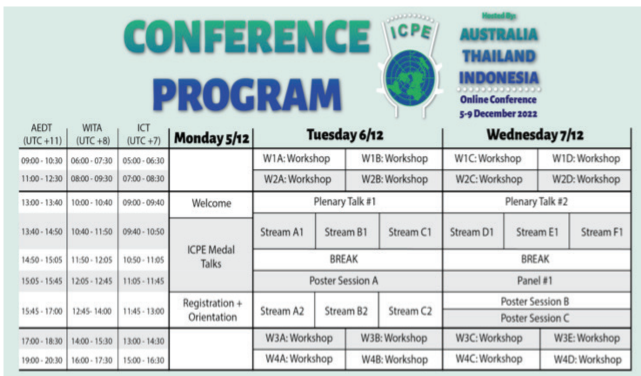


Figure 2: Technical team training session in week prior to conference.

them to refer to. We have placed our run sheets (created by Tom Dixon) on the conference website in case they are useful for other people planning a conference.

One thing we found surprising was the number of participants who needed a "participation certificate". As everyone was assigned a unique zoom name we were able to send participation emails to everyone who attended at least three zoom sessions during the conference and send pdfs to those who needed them.

Interactivity can be harder in an online conference, so we aimed to make our workshops as interactive as possible. We bookended the days with the workshops, scheduling them at times that were suitable for different participants (due to time-zones) and kept the numbers suitable for meaningful interaction, around 20 participants. We provided instructions to workshop facilitators encouraging them to include a number of interactive elements. These instructions are included on our website. This structure worked well, though did lead to long days for technical staff with workshops starting at 9 am and ending at 9 pm.



AEDT (UTC +11)	WITA (UTC +8)	ICT (UTC +7)	Monday 5/12	Tuesday 6/12			Wednesday 7/12		
09:00 - 10:30	06:00 - 07:30	05:00 - 06:30		W1A: Workshop	W1B: Workshop		W1C: Workshop	W1D: Workshop	
11:00 - 12:30	08:00 - 09:30	07:00 - 08:30		W2A: Workshop	W2B: Workshop		W2C: Workshop	W2D: Workshop	
13:00 - 13:40	10:00 - 10:40	09:00 - 09:40	Welcome	Plenary Talk #1			Plenary Talk #2		
13:40 - 14:50	10:40 - 11:50	09:40 - 10:50	ICPE Medal Talks	Stream A1	Stream B1	Stream C1	Stream D1	Stream E1	Stream F1
14:50 - 15:05	11:50 - 12:05	10:50 - 11:05		BREAK			BREAK		
15:05 - 15:45	12:05 - 12:45	11:05 - 11:45		Poster Session A			Panel #1		
15:45 - 17:00	12:45- 14:00	11:45 - 13:00	Registration + Orientation	Stream A2	Stream B2	Stream C2	Poster Session B / Poster Session C		
17:00 - 18:30	14:00 - 15:30	13:00 - 14:30		W3A: Workshop	W3B: Workshop		W3C: Workshop	W3E: Workshop	
19:00 - 20:30	16:00 - 17:30	15:00 - 16:30		W4A: Workshop	W4B: Workshop		W4C: Workshop	W4D: Workshop	

Figure 3: Program for first three days of conference, workshops were in the morning and evenings.

Emerging trends in physics education

Much of the conversation at the conference centred on a few key themes that are discussed below.

There are an increasing number of researchers looking into **student well-being** and how they feel in the classroom. From psychology literature, self-determination theory, it is well established that people (and students are people) have three psychological needs [1]:

1. Autonomy – some control over their situation, can be addressed by giving students choice.
2. Competence – opportunity to become very good at something and master the material.
3. Relatedness – need to feel like they belong to the community.

Many of the talks and workshops looked at how these needs could be addressed in different contexts.

The proliferation of online resources during COVID-19 lockdowns means that it is now much easier to give students choice about how they learn, increasing their autonomy. A number of talks looked at giving students more control over how they were assessed.

Many talks considered how to make students more effective and competent problem solvers. Again, online resources offer many opportunities in this realm. Students can use online question banks to practice answering questions numerous times, receiving constructive feedback as they go. Many talks focussed on how to achieve this in different areas of physics.

The importance of building students' sense of belonging was addressed in many talks, including the plenary talk by Prof. Chandralekha Singh. This is especially important for minority students, which in physics includes female students. In order to improve the gender balance and the learning experience of all students it is important to speak to them in a way that builds rather than destroys their sense of belonging to the physics community. Ways that this can be achieved were addressed in workshops and talks. A. Prof. Kate Wilson presented an interesting talk outlining some of the things we should keep in mind when setting assessments to ensure we are not inadvertently disadvantaging female students in our classes.

Online tools can offer effective ways to address student's needs for competence and autonomy. There were many talks and workshops demonstrating the use of different online tools. With the recent emergence of ChatGPT (which was too recent for discussion at this conference) online tools are and continue to be a game-changer in education. A number of different technologies were discussed.

Dr Derek Muller (Veritasium) discussed the use of videos for online learning. How to create and effectively use videos in teaching was a common theme among other talks in the conference as well. Using videos to present some concepts to students can be an effective way to free up class time for more active learning activities such as discussions and problem solving.

Laboratory learning was also a theme of numerous talks and workshops at the conference. Dr Sebastian Staaks, the creator of Phyphox gave an invited talk on how smartphone apps can be used to take readings of many phenomena, such as the angular velocity and acceleration of a bicycle wheel. The increasing availability of apps such as this to students opens up possibilities for students to be able to collect data outside of physics labs, possibly giving them more autonomy over what lab exercises they perform.

Other useful online tools and resources that were discussed at the conference included: the PhET and CoSci simulations and how they can be effectively embedded into courses; PhysPort, an incredibly useful resource for finding out about evidence-based best practice in physics; and virtual reality. Online tools also have their place in higher year physics courses, one of the workshops – held as a memorial to Ian Johnston - looked at how this could be achieved in Computational Physics. The emphasis of the workshop was on the tricky balance between physics, modelling and coding. Students need to know sufficient coding, or be taught within the course to be able to analyse and model specially selected problems which maybe broader than physics; real life problems. The coding language needs to fit within institutional structures. The benefit is developing 21st Century skills as well as computational thinking.

Teacher training. Many of the pressures felt by higher education are first felt in high schools. In her plenary talk Prof. Nam Hwa Kang talked about the expectations of Generation Z (zoomers) around education and how we can meet these expectations by using online tools and ensuring we are making use of active learning pedagogies. One of the themes that emerged in the high school space was how to ensure there is a balanced and interesting high school curriculum that has the right amount of content to give students a little autonomy over how the run their classes and allow space for active learning.

There were also many interesting uses of technology in the outreach domain, the ubiquity of online platforms now makes it much easier to reach students in remote schools.

Conclusion

We hope that many of you are able to make it to an education conference this year or the education stream at the AIP meeting. With technology advancing so quickly it is important that we all think carefully about how and what we are teaching our students and learn from each other about what works, what does not work and what possibilities new technologies make available to us.

About the author

Elizabeth Angstmann is a professor, education focussed academic and first year director in the school of Physics at UNSW. Liz won the AIP Education medal in 2020. Liz was the conference chair of ICPE 2022.

Jacinta den Besten is a Senior Lecturer in the School of Physics at the University of Melbourne. She is the Director of First Year Physics and was on the organising and program committee and chaired the Technical committee for the conference.

Thomas Dixon is an Associate Lecturer (Education Focused) in the School of Physics at UNSW. He is the first year lab director in the School. Thomas managed the technical staff and co-ordinated much of the technical aspects of the conference.

Manjula Sharma is a Professor of Science Education and Director of the STEM Teacher Enrichment Academy. She has co-founded the Australian Conference on Science and Mathematics Education and International Journal of Innovation in Science and Mathematics Education and has been awarded the 2012 AIP Education Medal, 2013 Australian Learning and Teaching Fellowship, 2019 STANSW Dedicated Service Award and is a Principal Fellow of the UK HEA, Fellow of AIP and Honorary Fellow of Teacher's Guild of NSW.

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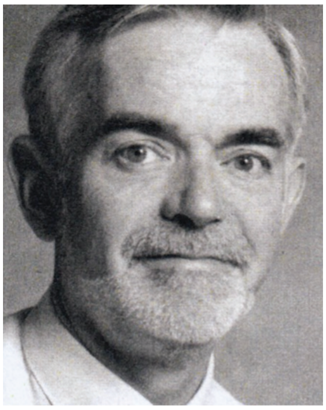
Remembering Ian D. Johnston

Helen Johnston (h.johnston@sydney.edu.au) and Manjula Sharma, School of Physics, The University of Sydney

Associate Professor Ian Desmond Johnston, a physicist and educationalist, died in December 2020 at the age of 83, leaving an enduring multifaceted legacy. The most remarkable aspect of Ian's career was his dedication to 'communities of practice' and passion for 'cutting edge computational technologies'; serving to better education. He remained largely invisible to those he was serving and will continue to serve long after he has gone. A life to celebrate!



Upon completing his schooling in Queensland, Ian commenced his PhD at The University of Sydney in 1960 under the supervision of Stuart Butler. He was one of the early users of SILLIAC, the first computer in Australia fired by valves which took up the entire basement of the School. While his thesis was on computational modelling of astrophysical problems, his most profound contribution to fundamental physics was research undertaken as a side project helping post-doctoral fellow Tetsuo Hamada. Prompted by giants such as Hans Bethe, Edwin Salpeter and Gregory Breit they carried out numerical calculations on nucleon-nucleon potentials. Thus, was born the *Hamada-Johnston potential*[1] published in 1961. The potential has a relatively simple analytical form and is extremely accurate, attracting considerable attention in the field of nuclear physics at the time. The paper is catalogued as a "Citation Classic", with over 1500 citations and continues to be cited a dozen times or so each year.

In 1964 Ian was appointed a Lecturer in the School of Physics during the Harry Messel Era; an Era when the School was being built up to be a great research and teaching institution. With the higher education sector still reeling under the "Wyndham Scheme" changes to high school teaching, Ian found himself in the midst of a backlash against television lectures, which were the source of much angst. Director of First Year Studies, Brian McInnes charged a team to rejuvenate the lecture series for the year-long Physics 1 Life Sciences course. Ian, working with John Lehane, remade the 50 minute television lectures on Quantum and Nuclear Physics. Taking on his hallmark research-based approach to teaching and learning, Ian viewed television as 'cutting edge computational technology' for solving a problem, rather than filming a lecture being delivered with chalk and talk interspersed with lecture demonstrations. Instead, his television lectures were innovative and exciting, with close-ups, action shots and location shots. He spent a year at the Open University in England, learning about other non-traditional ways of teaching.

Ian's interest in using technology to solve problems had already been piqued by using 'cutting edge computational technology' in the form of SILLIAC during his PhD; this interest flowed into his teaching. From here on, Ian devoted himself earnestly to education, focusing on technology as an enabler for learning.

In the late 1980s, Ian was captivated by the personal computer as a rapidly developing 'cutting edge computational technology' to benefit student learning, particularly in abstract topics where there was an interplay between mathematical formulation and visualization. He began a collaboration with Joe Redish at the University of Maryland, who had developed the MUPPET toolkit[2] (Maryland University Project for Physics Educational Technology). Fred Goldberg, working on 'everyday thinking' was also influential in matters of curriculum. During this collaboration, the concept of Computational Physics as a module run in parallel with lectures on quantum mechanics was formalized and content developed. The idea was that while some topics could offer hands-on experiments, others could have computational labs. Hence, lectures had a complementary activity, computational or experimental.

In 1989, Ian introduced a trial of computational physics into second- and third-year physics [3], in a variety of subject areas (quantum mechanics, non-linear oscillations, kinetic theory). He showed that the use of computers in physics instruction is not only possible but beneficial, with students able to tackle a wider variety of problems that can be approached in a typical lecture course. After the success of this initial trial, computational physics was rolled out permanently in second- and third-year courses, where it has remained a key part of the curriculum ever since. As languages changed from visual basic, to matlab and python, and operating systems changed, the modules have been updated. While Ian spearheaded and championed the initial stages, he was also instrumental in garnering a 'community of practice'; peers in the School bought-in and took stewardship of computational physics.

Ian's attention turned to sharing what he had learnt and advancing the potential capability of 'cutting edge computational technologies' to enhance or even transform physics education more broadly. In 1993, Ian used an Excellence in Teaching Award to finance the first Australian Computers in University Physics Education (OzCUPE) at The University of Sydney. This gathering, a 'community of practice', brought together like minded folk, with overwhelming call for more.

Over time, the OzCUPE conferences became affiliated with the Australian Institute of Physics (AIP) Congresses, to the extent that by 1998, the 4th OzCUPE was running in parallel with other significant affiliated conferences. The 5th and last distinct OzCUPE ran in 2000 at the 14th AIP Congress at Adelaide University with Judith Pollard as Chair.

However, the community hungered for more; to share practices through show-and-tell, learn about research based approaches, seeking to go beyond 'cutting edge technologies'. Hence, OzCUPE morphed into the AIP Physics Education Group (PEG). Strategically, Ian (working with Judith), persevered in gaining legitimacy and embedding PEG by establishing PEG as a formal Topical Group which AIP members can opt into. Furthermore, Ian and Judith were instrumental in creating the AIP Education Medal, a PEG 'stream' at AIP biennial congresses, as well as initiating PEG plenaries (the first of which was in 2000 [4]).

While the AIP had sought to create an education group from way back in 1956 [5], it wasn't till Ian's foresight in creating OzCUPE and connection with Judith that the 'community of practice', Physics Education Group, AIP PEG, in its current form was born.

In 1992, Brian McInnes led a group establishing SUPER, the Sydney University Physics Education Research group, with Ian spearheading a manifesto [6] which continues to guide the community. When Brian retired as Head of SUPER in 1994, Ian took on the leadership role. Under Ian's leadership, SUPER achieved a world-wide reputation for excellence. Ian supervised the first and second physics education research graduates in Australia, Kirsten Hogg in 1999 and Peter Fletcher in 2004 respectively. Capitalising on his international links, Ian facilitated the Chautaqwa physics workshops in Sydney, setting up an enduring partnership with Ron Thornton, famed for Interactive Lecture Demonstrations (ILDs). Ian led the drive for real time computational data taking and small group discussions in large lectures, active learning [7]. Ian's romance with communities around 'cutting edge computational technologies' continued.

The 1990's saw the internet open up for education; another opportunity for 'cutting edge computational technologies'. When the Government announced funding to setup subject area software clearinghouses, with the aim of evaluating, curating and promoting the use of new technologies in undergraduate science teaching across Australia, Ian rose to the challenge. Working with Mary Peat, they setup UniServe Science in 1995, including a journal and a conference. Under Manjula Sharma's stewardship, they continue as Australian Conference on Science and Mathematics Education (29th ACSME in 2023) and International Journal of Innovation in Science and Mathematics Education (Vol 31 of IJISME in 2023).

Ian's Directorship of UniServe saw him further extend his international engagement, with fruitful collaborations with Thai scholars and Commission C14, Physics Education of the International Union of Pure and Applied Science (IUPAP). Ian served as Chief Editor of C14 the Newsletter.

Throughout his whole life, Ian was also a dedicated and inspirational teacher. He was a frequent contributor to the Science Show on ABC radio. He turned his multi-episode show on the physics of music into a general textbook on music, called "Measured Tones, The Interplay of Physics and Music", first published in 1989, in its third edition and still selling today.

After his retirement in 2000, he remained an emeritus member of SUPER, working with Manjula in continuing to guide and inspire students who have gone onto diverse and successful careers.

We celebrate Ian through the enduring communities of practice he created and his keenness to be amongst the first to embrace 'cutting edge computational technologies' to benefit teaching and student learning. He leaves a legacy which has impressed many who know him, many who have not met him, and will continue to influence generations.

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An undergraduate physics student challenge

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In the depths of the COVID lockdown I ran into an intriguing problem in my research in nonlinear optics that did not yield to standard approaches. Though I solved it numerically, I suspected that there was more to it than I had found. Since the problem was relatively easy to state, I decided to set it as a challenge to undergraduate students. The quality of the responses was excellent—many of the students used a similar approach as I had, as had two of my colleagues, though some had been more systematic. However, the winners well exceeded my expectations. They found that the problem had been solved in the mathematics literature, in a different context, more than 50 years ago and that the solution cannot be written in closed form. Setting the Challenge and reading the submissions was satisfying and was a great way to engage with our top-students during a tough period. It also solved a problem that I had been struggling with.

Introduction

Many of us are encouraged, I suspect, to include aspects of our research in our undergraduate teaching to enhance the student experience. The student Challenge can be considered a variation on this—it was a difficult research-driven problem that was not suited for inclusion in a standard course. I therefore decided to make it a stand-alone item that would challenge the students outside their direct course work. Here, I briefly describe the Challenge, its solution and what I learned.

Context

My research is in nonlinear optics. Nonlinear optical effects occur when the light intensity is so high that the refractive index of a material depends on the electric field strength, and thus on intensity. My colleagues and I developed a fibre laser over the last few years in which the dispersion, the dependence of the (effective) refractive index on frequency, can be freely chosen by a programmable spectral pulse shaper [1]. At sufficiently high powers, this laser acts nonlinearly and can emit a wide variety of soliton pulses depending on the dispersion [1,2,3]. The Challenge arose in the context of the investigation of solitons that consist of multiple frequency components [3]; in our experiments we generated solitons with up to $J = 5$ components (Fig. 1(a)-(d)). The frequency components, which arise purely from phase effects, travel at the same group velocity and are coherent. They therefore beat in the time domain, leading to optical pulses (Fig. 1(e)-(h)) which consist of a slowly varying envelope (indicated by the dashed curves in Figure 1), multiplying a strongly modulated carrier.

We developed a theory that accompanies these experiments. This is a theory for the electric field envelope of the pulses, which depends on the carrier, i.e., the amplitudes of the frequency components. This theory shows that these pulses have interesting and useful properties. To appreciate these you need to know that nonlinear optical effects tend to be weak and that they therefore often need to be enhanced. For this reason almost all nonlinear optics experiments are carried out in waveguides, which allow long propagation lengths. The waveguides are typically designed such that the light is strongly confined in the direction *transverse* to propagation [4]; this requires small waveguide cross sections and a large refractive index contrast. The light can be confined in the direction of propagation by reducing the group velocity ("slow light") [5].

Returning to Fig. 1(e)-(h), in the nodes the intensity vanishes and thus so do the nonlinear effects. But at the antinodes the intensity is enhanced and so are the nonlinear effects. The nonlinear optical effects increase superlinearly with the electric field strength, so the enhancement of the nonlinear effects at the

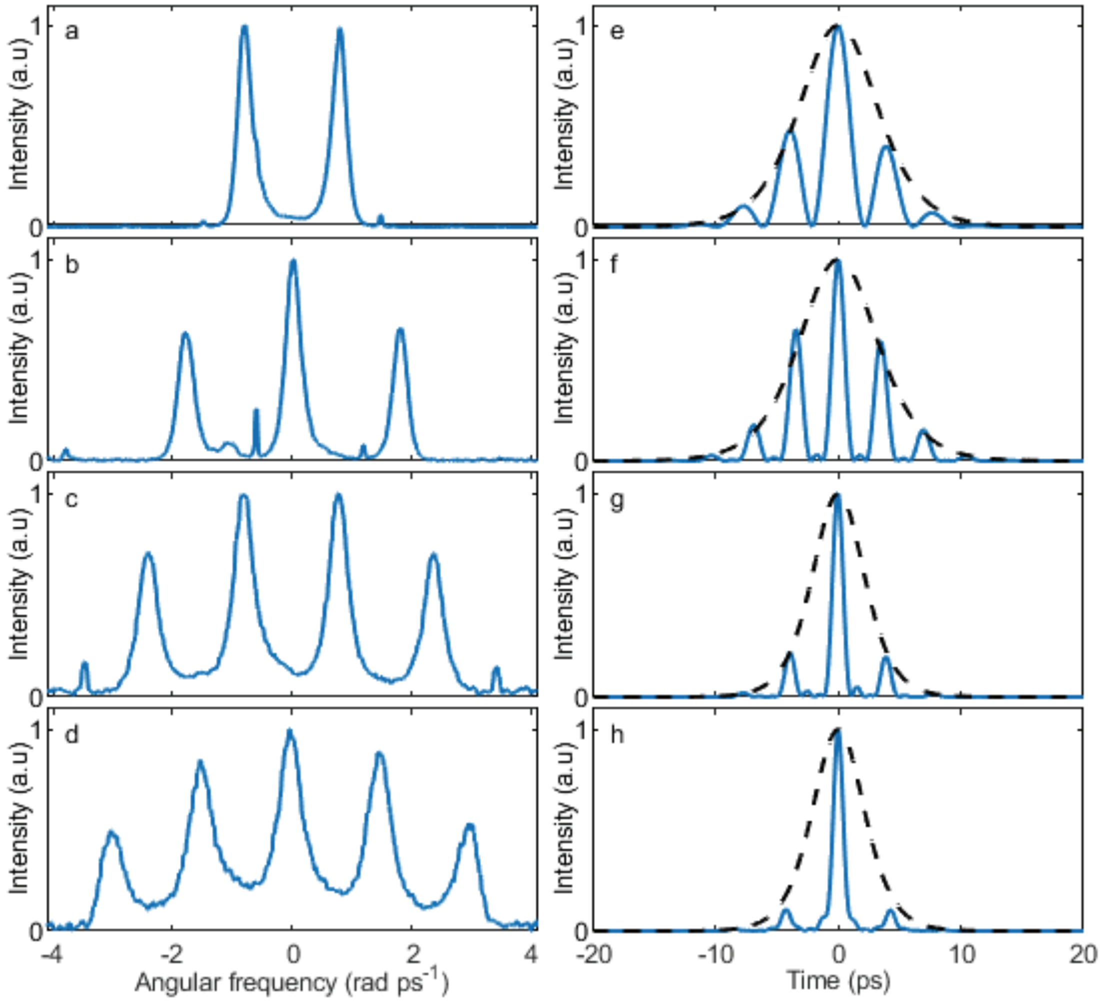

Figure 1: (a-d) Measured pulse spectra for $J = 2, \ldots, 5$ frequency components. (e-h): Measured temporal pulse shape associated with the spectra in (a-d).

antinodes more than compensates for the drop around the nodes, and thus the overall strength of the nonlinear effect increases. For example, for two frequency components the nonlinear effect is $\mathcal{E}$=1.5 × larger than for a pulse consisting of a single frequency component of the same duration. For five frequency components the enhancement is $\mathcal{E} \approx 3.5$ [3].

Introduction to the Challenge

The Challenge hinges on the relative amplitudes of the frequency components in Fig 1 which follow from their nonlinear interactions. These can be calculated as follows: let the frequency components have amplitudes p_j, with j between $\pm(J-1)/2$ where J is the total number of components. The p_j are real and $p_{-j} = p_j$. Though I have implicitly taken J to be odd, for even values the results are similar. The set of amplitudes $p_{\{j\}}$ can then be found as follows [3]

(i) Convolve the $p_{\{j\}}$ with themselves three times. i.e. let $q_{\{j\}} = p_{\{j\}} \times p_{\{j\}} \times p_{\{j\}}$, where × indicates a convolution.

(ii) Truncate the $q_{\{j\}}$ so that it has the same number of components as the $p_{\{j\}}$.

(iii) Choose the $p_{\{j\}}$ such that q_j/p_j is independent of j. The nonlinear enhancement is then $(q_j/p_j)^2$.

For example, for $J = 3$ after the convolution and truncation we have $q_{\pm1} = 3p_{\pm1}^3 + 3p_{\pm1}p_0^2$ and $q_0 = p_0^3 + 6p_0p_{\pm1}^2$. This gives $p_{\pm1}/p_0 = \sqrt{2/3}$ and an enhancement factor of $\mathcal{E} = 15/7$.

For higher values of J this procedure becomes increasingly tedious and requires solving a high-order polynomial. Moreover, it does not provide an overarching understanding. Is there some underlying functional form for the frequency components? What can be said about the nonlinear enhancement as the number of frequency components grows?

We did establish that the p_j are those that lead to the highest nonlinear enhancement $\mathcal{E}$. In other words, the system operates such that $\mathcal{E}$ takes its maximum value.

The Challenge

The Challenge was in essence the continuum version of the discrete problem discussed above, which centred around the function $f(j)$ (though it was written as $f(x)$ in the Challenge document). It took a while to define it such that it was unambiguous and straightforward to explain. The final formulation can be seen in Figure 2. The students were given about a month to submit their solutions. Notice that the Challenge can be straightforwardly stated and that the amount required mathematics to make some progress is modest. I distributed it to physics and mathematics students at the University of Sydney via the respective student societies, and also sent it to colleagues at Macquarie University, UTS and at the University of Auckland for distribution to their students.

Solution to the Challenge

In the end I received seven independent submissions. Some students had worked alone though most had worked in pairs. Informal discussions with other students showed that more had worked on the Challenge but had unfortunately deemed their solution to be of insufficient quality to be submitted.

Most submissions consisted of a trial function, or a set of trial functions, for $f(x)$, typically an even order polynomial, and then choosing the coefficients such that the nonlinear enhancement factor $\mathcal{E}$ was a maximum. Some gave a large number of decimal places, the first seven of which are $\mathcal{E}= 0.6869813$.

The students behind the winning entry had gone a step further. They posted the problem on the bulletin board Mathematical Stack Exchange, where it was suggested that they enter the number 0.68698… into the Google search engine with varying numbers of decimal places. They struck gold and found the paper entitled "On Some Extremal Positive Definite Functions" by Garsia *et al*, published in 1969 [6]. Garsia *et al.* in essence solved the same problem, though phrased differently, with complete mathematical rigor. Briefly, they considered, in our notation, a continuous function $a(x)$ with a nonnegative Fourier transform and $a(0) = 1$ and $a(x) = 0$ for $|x| > 1$. Given those constraints, what is the largest possible value $\int_{-1}^{1} |a(x)|^2 dx$?

The authors mention that their "... question has arisen in trying to maximize the average power of the received signal in the radar exploration of the planets carried out at the Jet Propulsion Laboratory." They prove that there is a unique maximum, they develop an iterative procedure for finding the optimum function that converges geometrically, give $\mathcal{E}$ to 24 decimal figures and they find exact value for $f(\pm {}^1/_2)$. The authors comment that "It would be interesting if (the solution) could be expressed in terms of familiar functions or if ($\mathcal{E}$) itself turns out to be related to some of the classical constants." The students addressed this problem using the technology available to us today but found that the value of $\mathcal{E}$ appears not to be related to any other mathematical constant. A forward literature search showed that the problem is quite a general one and that it is related to various optimisation problems and even to the statistics of the largest eigenvalue of certain random matrices [7].

For the record, $f(x)$ can be approximated as $f(x) = 1 + b_2x^2 + b_4x^4 + b_6x^6 + b_8x^8 + \cdots$ with $b_2 = -1.79024$; $b_4 = 1.10688$; $b_6 = -0.34723$; and $b_8 = 0.06584$.

Discussion and Reflection

This was truly a research-enriched undergraduate experience; the Challenge engaged some of the students even during a COVID lock-down and my anecdotal evidence is that they enjoyed it. I thought the considerable time I devoted to describing the problem plainly and unambiguously was time well spent—the last thing you want to do is to send corrections out.

One of the main decisions was whether to state the problem in the time domain or in the frequency domain. I tried both and decided that the frequency domain was the better choice. Working with the physics student society was a good move and helped me reach a large group and gave me a forum when announcing the winners. While one does not run every day into suitable problems like this one, namely, which can be stated easily; which at least can be attempted by undergraduate students, it is good to keep this in mind. What did I learn? Well, first of all, never underestimate the creativity of a good student. Moreover, it was reassuring to know that the problem was indeed a "difficult" one. One might argue that this is mathematics problem rather than a physics one. However, this is the problem I encountered; it would be interesting to conceive of an experiment that could be done safely at home with standard household items. What would I have done differently? I think it was good to try and get other universities involved, but I was somewhat too casual about it. All submissions came from the University of Sydney; rather than working via colleagues I should have worked via the local physics student societies. On the other hand colleagues at other universities made submissions but I deemed them ineligible (and their submissions were not as good as that of the winners!). I also have a renewed appreciation for the sophistication of Google's search algorithm.

The winners, Georgio Hawi and Sharvil Kesarwani reflected "This all began as a challenge, set by Martijn to our university's physics society members, where we were asked to solve a particular constrained optimization problem over classes of functions. This problem was very simple to state, yet very difficult to solve. In the process of doing so, we enhanced our understanding of a variety of techniques and approaches, including Fourier analysis, the Euler-Lagrange equations, and numerical methods. We were interested to find that this problem has physical relevance in the field of optics, where the quantity maximized corresponds to the nonlinear enhancement factor of a light pulse."

All students received a physics society t-shirt and the winners are co-authors on a publication [8] which includes the outcome of this challenge—it has been great working with them on this!

Acknowledgements

I'd like to thank all the students who participated in the Challenge and colleagues for giving useful feedback., in particular A/Prof. Tristram Alexander. I thank Joshua Lourdesamy for providing me with Figure 1.

About the author

Martijn received the Ingenieur degree from the University of Delft and a PhD from the University of Rochester. After postdoctoral work at the University of Toronto in Canada he joined the University of Sydney where he is now a Professor in Physics. His research area is optics and photonics with more recent adventures in atmospheric water capture and the dynamics of light sails. Most early mornings you can find him in the local pool swimming laps.

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Student challenge

Martijn de Sterke

September 6, 2021

Consider a real, symmetric function $f(x)$ that is nonzero only for $-1/2 \leq x \leq 1/2$ and for which $f(0) = 1$. Now apply the following construction to f:

- Take the autocorrelation $a(\Delta)$, i.e.

$$a(\Delta) = \int_{-\infty}^{+\infty} f(x) f(x - \Delta) dx,$$

  which is nonzero only between ± 1.

- Consider the quantity

$$\mathcal{E} = \frac{\left(\int_{-1}^{+1} a^2(x) dx \right)}{a^2(0)}.$$

- My question is: for which function f does $\mathcal{E}$ take its largest value and what is this value?

As an example consider the rectangle function

$$f(x) = \begin{cases} 0, & x > 1/2, \\ 1, & x < 1/2. \end{cases}$$

Its autocorrelation is the triangle function

$$a(x) = \begin{cases} 0, & |x| > 1, \\ 1 - |x|, & |x| < 1. \end{cases}$$

Following the procedure described above you then straightforwardly find that $\mathcal{E} = 2/3$. Can you do better?
This is a problem that has come up in our research in nonlinear optics. I think I know the answer but I have found it in a somewhat *ad hoc* way. I would be particularly interested in any insight as to why the optimal solution is indeed optimal and whether there is a constructive way to find it. Numerical results are of course also welcome.

Figure 2: The actual student challenge.

#PhysicsGotMeHere

The aim of this series is to highlight different career pathways for physics graduates. A different physics graduate is featured each month in our monthly AIP bulletin, and over our social media accounts and websites. The format is quite flexible – tell us your story with roughly the titles below. Read through other #PhysicsGotMeHere articles at https://www.aip.org.au/PHYSICSGOTMEHERE.

Thank-you very much for sharing your career story – we hope it will help our students and Early career members find a career that suits them!

Wilson Pok – Data Scientist at Google

'The ability to 'go deep' on a complex, technical topic is extremely valuable and transferable, and that is a skill that physics training provides.'

Where I work: Google

What I do: As a data scientist, I help businesses run and analyse large-scale experiments.

My physics background: Semiconductor physics. After I got my physics PhD, the field of data science started taking off, and the technical problem-solving skills that I had developed through physics set me up to be a good match for these roles.

How physics has helped me get to where I am: There are core skills that I use, like researching scientific papers on latest methodologies, and framing business problems as technical ones. Additionally, there are more specific skills, like statistics and programming, that I use every day.

When I started meeting other data scientists and found that many of them were also physics PhDs, I realised that this is actually a common career path.

Find me on: Linkedin.com/in/WilsonPok

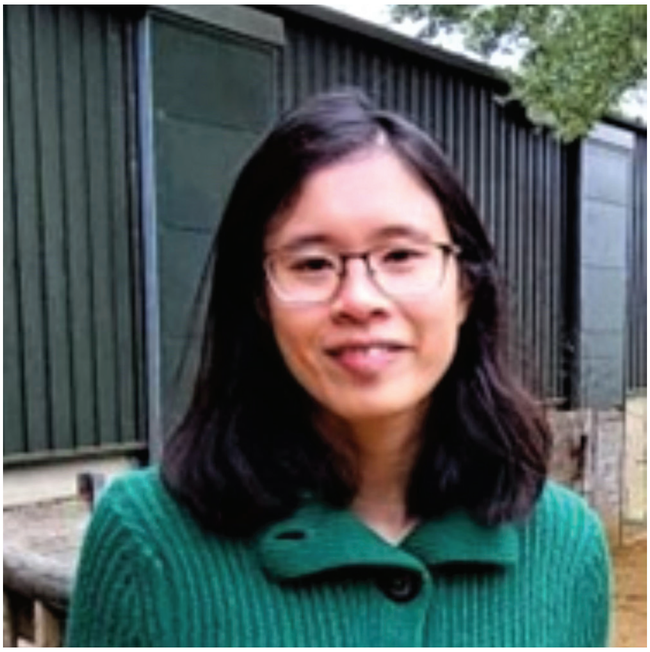
Ada Yan – Virologist at Imperial College London

What I do: I work as a virologist at Imperial College London. I study how bird flu adapts to humans, to better predict which bird flu strains might be likely to cause a pandemic.

My physics background: I completed my Masters in theoretical condensed matter physics, improving phase retrieval algorithms for electron microscopy.

How physics has helped me get to where I am: During my masters, it became apparent that while I enjoyed using mathematics to understand real-world phenomena, I would prefer other applications such as in biology. I applied for a few PhD positions in biophysics, before stumbling upon an ad posted in the physics department, for a PhD position in mathematical modelling of infectious disease in the School of Public Health. I was unaware that this field existed, but after meeting the team and doing some reading I was hooked. It turned out that the skills I had acquired in my MSc, such as describing real-world phenomena using equations, analysing data and coding, were applicable to mathematical modelling in other fields.

After my PhD, I took two postdoc positions in mathematical modelling of infectious disease and the immune response. I became increasingly interested in how the experimental data I was analysing was generated. I realised that if I were to one day lead projects and teams combining mathematics and biology, I would need to understand the world of biology more fully – which questions are at the cutting



edge, what new technologies might help us understand them, and how experiments are designed and performed. With support from my experimental collaborators, I applied for and received a fellowship, where I am performing my own experiments as well as analysing them using mathematical models.

In terms of technical skills, physics training gave me the analytic and computational tools required to analyse model equations and relate them to data. The spread of infectious disease, whether between individuals or within a host, is ultimately a physical process, and the equations describing these processes can be analysed using the same methods as in physics.

But more importantly, physics training began my journey in learning the research process – planning a research project, forming hypotheses, designing and refining experiments (in the lab or in silico), reporting results and forming new research directions. I have learnt to communicate new ideas with collaborators, form networks and develop resilience.

There has not been one particular moment, but during the pandemic it became apparent how researchers from all disciplines were required to solve problems in infectious diseases. The contribution of physics was invaluable, from understanding processes of aerosolisation, airflow and deposition to unravelling the structures of viral proteins.

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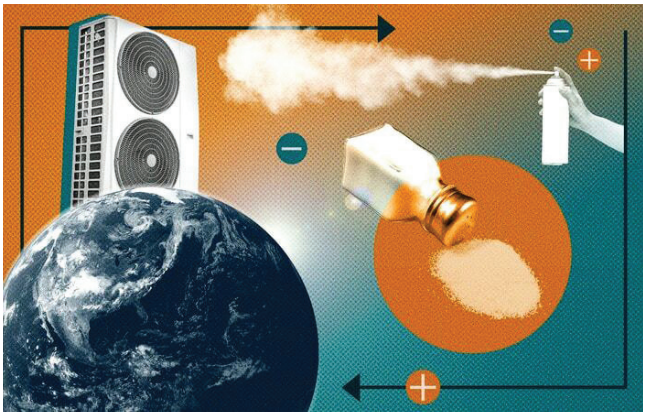
Physics around the world

Ionocaloric cooling makes a new type of refrigerator



Ionocaloric cooling could help phase out refrigerants that contribute to global warming. (Courtesy: Jenny Nuss/ Berkeley Lab).

A new refrigeration method dubbed "ionocaloric cooling" could one day replace traditional systems based on vapour compression, reducing the need for gases that harm the Earth's atmosphere and contribute to climate change. The method, developed by researchers at the Lawrence Berkeley National Laboratory (LBNL) in the US, takes advantage of the ways that energy is stored or released when a material changes phase, such as from a solid to a liquid or vice versa.

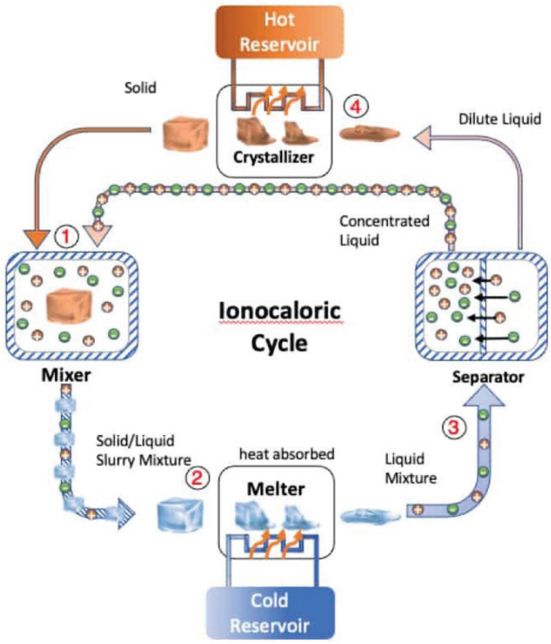
Conventional refrigerators and air conditioners are designed to use volatile hydrofluorocarbons, which are extremely powerful greenhouse gases with a global warming potential (GWP) 2000 times greater than carbon dioxide. In such systems, the refrigerant is pumped around a closed loop in which it undergoes a phase change from a liquid to a gas and then back to a liquid. The transition to a gas involves an expansion and requires energy, which the refrigerant acquires by cooling the surroundings on its "cold" side. Heat is then released on the "hot" side when the fluid condenses back to a liquid.

This standard cycle can also be applied to other substances that similarly undergo a phase transition involving the absorption and emission of heat. These alternative substances include electrocaloric and magnetocaloric materials, which switch between two solid phases in the presence of applied electric or magnetic fields. The drawback is that the heating and cooling abilities of electrocaloric and magnetocaloric refrigerants are relatively modest, leading to cooling cycles that are inefficient for widespread practical use.

A third possibility is to use the barocaloric effect, which occurs when the material being compressed and expanded is a solid rather than a liquid or gas. For most barocaloric materials, however, this effect is very small at ambient temperatures and pressures.

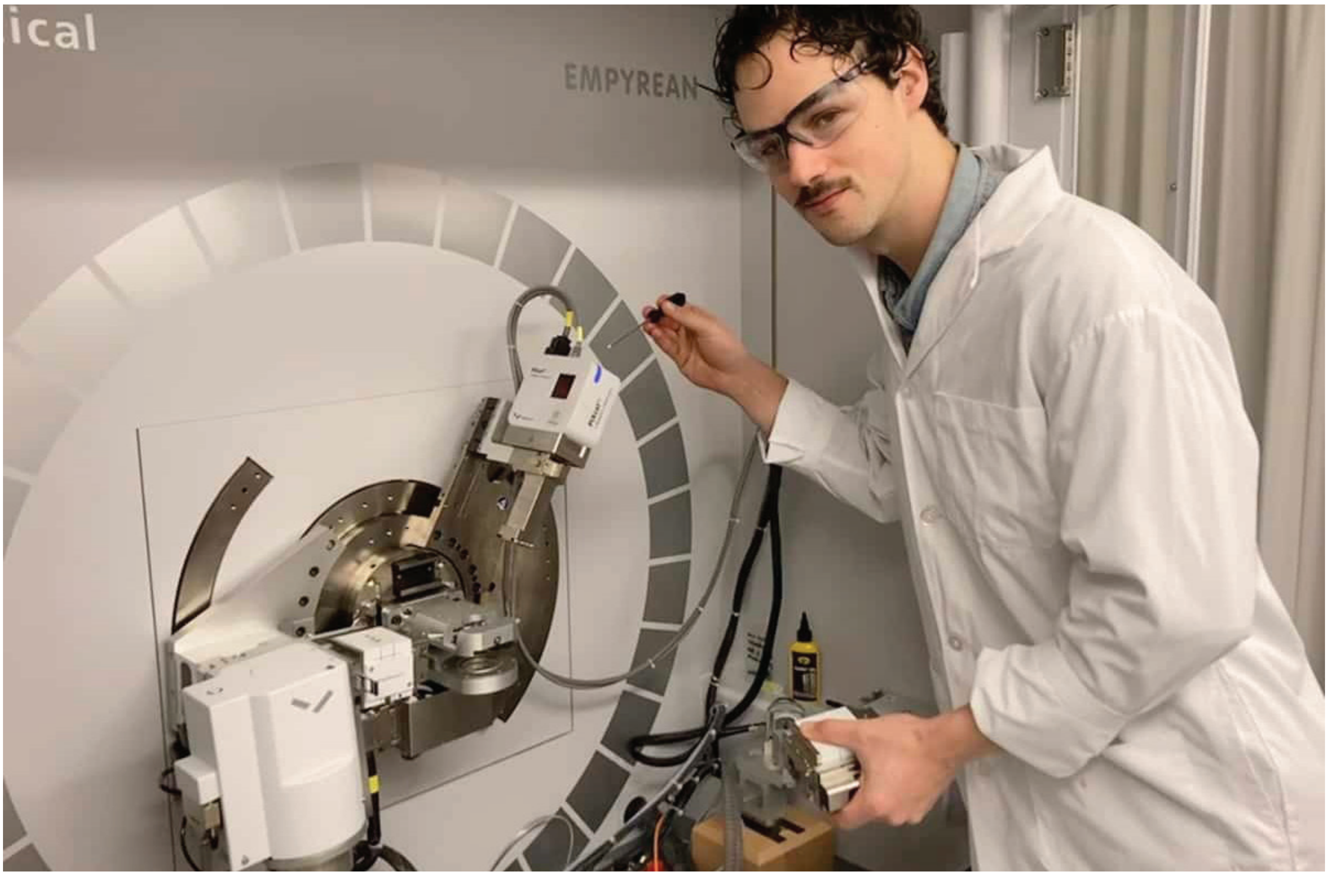
A completely new caloric effect

The new technique invented by Drew Lilley and Ravi Prasher at LBNL makes use of an entirely different caloric effect. It works by adding salt to a solid, which makes the solid "want" to be a liquid in the same way as adding salt to a cold, icy road transforms the ice into slush.



Salty ice: The ionocaloric cycle. (Courtesy: Drew Lilley/ Berkeley Lab)

"To become a liquid, the solid must melt, which means it must absorb energy," Lilley explains. "If you prevent the solid from absorbing energy from its surrounding, it will 'steal' energy from itself, so cooling the whole material down (see steps 1 to 2 in the image above). Once it has cooled down, the solid can continue melting, but at a lower temperature, and absorbs energy from its surroundings. This leads to refrigeration (steps 2 to 3 in the diagram)."



Optimized medical imaging Jericho O'Connell and colleagues at the XCITE Lab are investigating the use of high-resolution perovskite detectors in common X-ray imaging devices. (Courtesy: Jericho O'Connell)

A slow, salty cycle

The salt the researchers used is made from iodine and sodium, and they mixed it with ethylene carbonate – a common organic solvent that is, incidentally, a common additive in lithium-ion battery electrolytes. The resulting ethylene carbonate–sodium iodide (EC-NaI) mixture is, they say, CO2-negative, environmentally benign, non-hazardous, zero-GWP, nontoxic and non-flammable.

(extracted with permission from an item by Isabelle Dumé at physicsworld.com)

Could next-generation perovskite detectors improve clinical X-ray imaging?

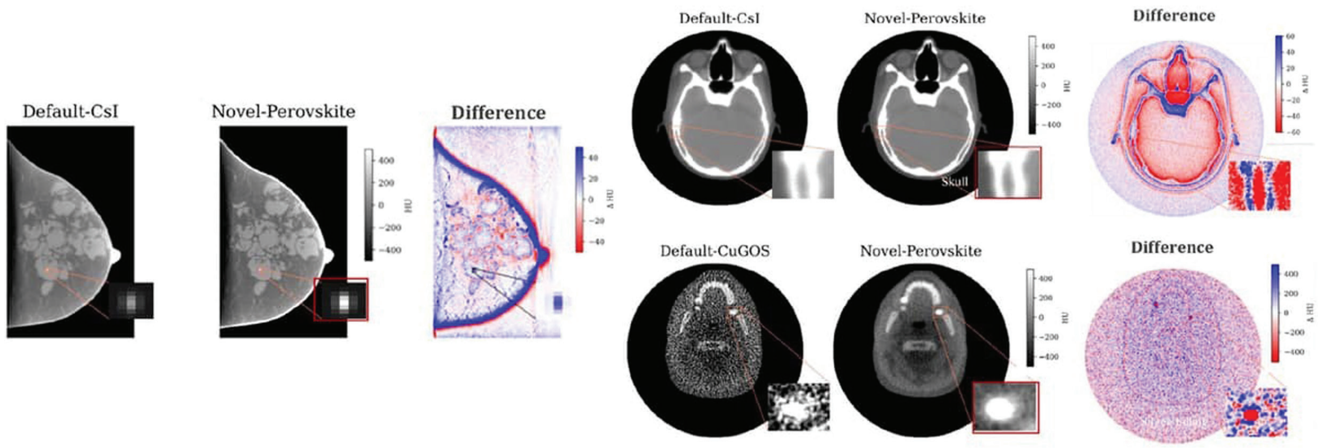
Perovskite-based X-ray detectors have a lot to offer the field of diagnostic imaging: low production costs, direct conversion, high absorption efficiency and superior spatial resolution to existing detectors. But while these advantages have been demonstrated in previous studies, researchers have not yet determined whether they translate to improvements in clinical applications.

To investigate this potential in more depth, researchers in the X-ray Cancer Imaging and Therapy Experimental (XCITE) Lab at the University of Victoria in Canada have performed virtual clinical trials on next-generation perovskite detectors integrated into common X-ray imaging devices, reporting their findings in Physics in Medicine & Biology.

The team investigated the perovskite crystal methylammonium lead bromide (MAPbBr3), which combines high charge carrier mobility and long carrier lifetimes, making it extremely sensitive to incident X-ray photons. Indeed, some MAPbBr3 crystals show equivalent performance to that of cadmium zinc telluride (CZT), a promising material used in cutting edge medical imaging techniques such as photon-counting CT.

To determine which imaging applications may suit perovskite detectors, the researchers used TOPAS Monte Carlo (MC) simulations to calculate the energy deposition efficiency (EDE, the fraction of absorbed energy relative to the incident energy) of MAPbBr3, for crystal thicknesses between 40 and 15 mm and beam energies from 20 keV to 6 MeV.

They compared the results with four other detector materials: amorphous selenium (a-Se), commonly used for mammography; caesium iodide (CsI), the standard detector material for kilovoltage (kV) CT; gadolinium



Virtual clinical trials Images of phantoms using default detectors and perovskite detectors for breast CT (left), kV-CBCT (top right) and MV-CBCT (bottom right). The difference images show regions where perovskite has higher HU values in blue. (Courtesy: Phys. Med. Biol. 10.1088/1361-6560/acae15)

oxysulphide (GOS), as used in kV and megavoltage (MV) imaging; and CZT.

Due to the lead content in MAPbBr3, the perovskite exhibited the highest energy absorption of all the detectors in the mammographic energy range. For MV imaging, only CZT had superior EDE, while for kV imaging, perovskite did not generally perform as well as the others. Based on these findings, the team chose three imaging systems to study: the Koning dedicated breast CT scanner, and Varian's Truebeam kV and MV cone-beam CT (CBCT) systems.

"The EDE simulations motivated the inclusion of breast CT, a more niche imaging system that we would not have simulated otherwise," explains first author Jericho O'Connell. "The kV- and MV-CBCT systems would have been included regardless, as they are key parts of the radiotherapy workflow."

Virtual clinical trials

O'Connell and colleagues used Fastcat hybrid MC simulations to optimize the perovskite detector design for each application. By maximizing the detective quantum efficiency (DQE, the efficiency of converting an input signal to an output image), they calculated the optimal thicknesses for the perovskite crystals as 0.30, 0.86 and 1.99 mm, for breast CT, kV- and MV-CBCT, respectively. They then used these device-specific detectors in a series of virtual clinical trials.

For the breast CT trial, the researchers simulated a breast phantom with microcalcifications imaged using the default CsI detector and a perovskite detector with the same pixel pitch (0.194 mm). The perovskite detector increased contrast in the microcalcifications by 87%, clearly visualizing a calcified lesion that was poorly defined using the CsI detector. This could enable more accurate identification of such structures in breast cancer screening when using a perovskite detector, which can be manufactured at lower cost than CsI.

In the kV and MV CBCT virtual trials, the researchers imaged an XCAT head phantom. In both cases, the perovskite detector dramatically improved image quality compared with the default detectors. In the kV images, spatial resolution in fine bone features and tissue contrast was improved dramatically using the perovskite detector, increasing the CNR in brain and skull by 8% and 13%, respectively, compared with the CsI detector.

The MV image focused on a skull region containing silver fillings that would generally produce large streaking artefacts in kV images. The high efficiency of the perovskite detector compared with a GOS detector resulted in dramatic improvement in CNR and enabled a metal artefact-free image of the jaw. The researchers point out that the improved contrast in MV-CBCT images with a perovskite detector could enable imaging of patients on radiotherapy machines without a kV on-board imager, as is the case for most systems in low- and middle-income countries.

Replacing the current detectors on the breast CT, kV-CBCT and MV-CBCT machines with optimized perovskite detectors improved the DQE of these systems by 12.1%, 9.5% and 86.1%, respectively. "Perovskite detectors perform better than current detectors in breast CT and kV-CBCT applications, and are far superior to current MV-CBCT detectors in terms of CNR and DQE," the researchers conclude.

(extracted with permission from an item by Tami Freeman at physicsworld.com)

PRODUCT NEWS
Coherent Scientific

Superconducting Nanowire Single Photon Detectors

Superconducting Nanowire Single Photon Detectors (SNSPD's) provide outstanding performance for quantum optics applications that require detection of single photons with high efficiency and superb timing resolution.

Single Quantum provides the fastest and most sensitive single photon detectors on the market. Their flagship EOS system consists of a compact closed-cycle cryostat, fibre-coupled SNSPD's, a user-friendly electronic driver, and the Single Quantum web-based software.

- Unparalleled system efficiency: >90%
- High count rate: >80MHz
- Low timing jitter: <15ps
- Low dark count rate: <10 Hz
- Sensitivity from UV to mid-IR
- Continuous operation with no helium required

New Advanced Optical Filters and Catalogue

The new Avant filter set family from Semrock has been designed to provide significant improvement in fluorescence performance for corresponding short Stokes Shift fluorophores.

IDEX Health & Science's new Semrock Avant technology narrows the gap separating excitation and emission passbands and brings passbands close together. The Avant family of sets therefore delivery significant increases in fluorescent signal, achieved by steep spectral edges and high OD blocking of the excitation passband in the emission filter.

The new 2023 catalogue is now also available for download from Semrock's website.

CW Ytterbium Booster Fibre Amplifier

The CYFA-BO series (Continuous Ytterbium-doped fibre amplifier) from Keopsys are designed for continuous operations in the 1.0 µm range. The amplifiers deliver up to 42dBm of saturated output power and are available in random or linear polarisation.

Several optical amplification bandwidths are available from 1029nm to 1114nm. The amplifier design is highly robust and is also designed to amplify narrow linewidth signals (<100kHz).

Applications include material characterisation, nanotechnology, quantum optics or nonlinear optics for visible light generation.

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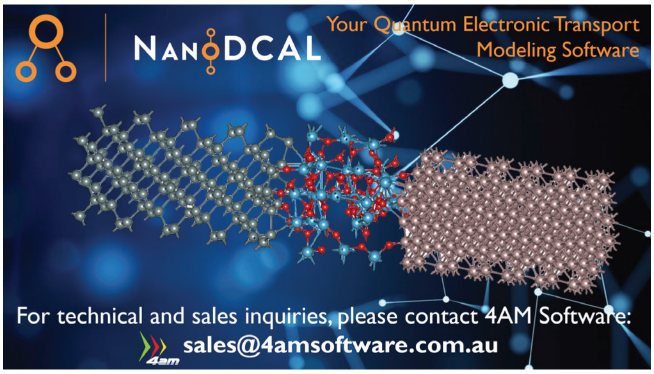
NANOACADEMIC Technologies

NanoDCAL

NanoDCAL offers reliable and powerful quantum transport simulation features to model nanostructures or nanodevices. It is an atomic orbital implementation of NEGF-DFT. It computes the Hamiltonian of materials and devices from first principles (i.e., without external parameters) using density functional theory (DFT) and simulates quantum transport phenomena within the Keldysh non-equilibrium Green function formalism (NEGF). NanoDCAL includes a large suite of methods for calculating important transport properties of your materials. NanoDCAL was used in hundreds of peer-reviewed papers in domains as varied as molecular electronics, nanotubes, topological insulators, batteries, magnetic tunnel junctions, metal grain boundaries (crystallites) and more: all of them can be found referenced on our website, under Technical Insights menu. It has demonstrated efficiency, so why not test it? Unleash the full power and functionality of NanoDCAL by obtaining a parallel license and use it at its full potential.



Main NanoDCAL features are the following:

- Written in MATLAB and C
- Focus on molecular and nanoscale electronics (small to large scale 1k+ atom systems)
- Spintronics (collinear / non-collinear / spin-orbit coupling)
- Semiconductor nanoelectronics (I-V curve)
- Several features such as total energy, force, scattering states and phonons calculations are part of NanoDCAL suite
- Study molecules, crystals, one-probe and two-probe systems
- Force, stress, structure optimization
- Electron-phonon coupling
- Atomic orbital basis optimizer
- Photocurrent
- Thermal transport coefficients

We offer licenses for single users and research groups and some options such as the HPC (parallel version) and advanced training and support services.

A free trial version is available for testing. Create your free user account today and start using our advanced atomistic tool, today!

RESCU

RESCU – Real space Electronic Structure CalcUlator – is a powerful MATLAB-based density functional theory (DFT) and DFPT (perturbation theory) solver. It can predict the electronic structure and derived properties of bulk materials, material surfaces and molecules. RESCU calculates the ground-state density using a basis of numerical atomic orbitals, plane-waves or real space grids, or a combination of them. Written with the objective of solving systems comprising up to a few tens of thousands of atoms, RESCU is carefully parallelized and exploits libraries such as MPI, ScaLAPACK and CUBLAS. It includes many state-of-the-art analysis tools such as density of states (DOS), projected density of states (PDOS), local density of states (LDOS, PLDOS), finite-displacement phonon and band structure. It has some unique features that most if not all other commercial codes on the market do not have.

Main RESCU features are the following:

- Written in MATLAB and C
- Focus on large scale systems (up to 20k atoms)
- DFPT implementation (e.g., dielectric tensor, dynamical matrix)

- Optical properties (e.g., dielectric permittivity, refractive index)
- Raman tools (e.g., tensor, spectrum, intensities)
- Advanced functional treatment such as DFT + EXX (hybrid) and DFT + U (Hubbard)
- Common analysis tools like DOS, PDOS, LDOS, PLDOS, band structure, band-unfolding, charge analysis
- Non-linear optical susceptibility
- Spintronics (collinear / non-collinear / SOC)
- Phonon tools (finite-difference-based)
- Large scale CFSI solver

We offer licenses for single users and research groups and some options such as the HPC (parallel version) and advanced training and support services.

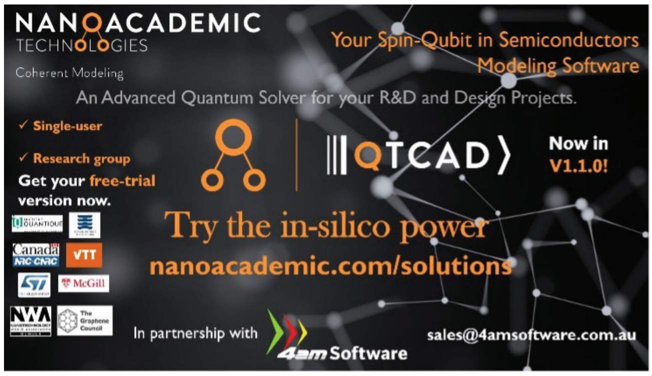
A free trial version is available for testing. Create your free user account today and start using our advanced atomistic tool, today!

QTCAD

Nanoacademic Technologies Inc.'s QTCAD newly released software is unique on the market and enables to study arbitrary gated quantum dot configurations in semiconductors including for example advanced III-V alloys such as GaN and AlN (Nitride) materials, but all semiconductors can be studied. QTCAD is the only commercially available computer-aided design software with all the features needed to model spin qubits in gated quantum dot devices, namely, device electrostatics at cryogenic temperature, single-particle Schrödinger solvers for electrons and holes within k.p theory, and quantum-mechanical many-body solvers accounting for Coulomb interactions within the gated quantum dots. QTCAD simulations have recently been used in the interpretation of experiments with industrially fabricated gated quantum dot devices such as FD SOI architectures.

Main QTCAD features are the following:

- An interface with our large scale DFT software RESCU (k·p theory)
- An electrostatics tool that solves the confining potential of quantum dots in semiconductor
- A valley-splitting calculation tool;
- An exact diagonalization tool / many-body Schrödinger solver for electrons and holes;
- A master equation solver for quantum transport calculations in the sequential tunneling regime enabling treatment of Coulomb blockade and predicting charge stability diagrams;



- Quantum-mechanical treatment of magnetism (orbital and Zeeman effects);
- Linear spin-orbit coupling from arbitrary user-defined Hamiltonians;
- Our electric-dipole spin resonance module interfaces with QuTiP for time-dependent simulations of quantum control;
- Works at cryogenic (sub-K) temperatures in many practical designs of solid-state spin qubits, which is a notoriously difficult problem to solve with available TCAD software;
- Arbitrary 1D, 2D and 3D device geometries are defined via Gmsh using our adaptive meshing technique to avoid time-consuming manual mesh refinements. Simulations are launched using our user-friendly Python API.

Many more features are in the works to extend the reach of QTCAD over quantum technologies and more physics phenomena. We offer licenses for single users and research groups and optional advanced training and support services.

QTCAD is now commercially available for academic users, a Professional version will launch soon (companies: please contact us for more information on info@nanoacademic.com).

A free trial version is available for testing. Create your free user account today and start using our advanced quantum modeling tool, today!

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Visit us for more technical descriptions on our website www.nanoacademic.com and linked documentation: https://docs.nanoacademic.com/.

For any commercial inquiries, please contact our ANZ Partner 4AM Software on sales@4amsoftware.com.au

Scitek

HiPace® 80 Neo

The Pfeiffer HiPace 80 Neo turbopumps are compact yet powerful operating at pumping speeds of up to 67 l/s for N2.

Enjoy the compact design which offers minimum footprint. No matter what gasses you are working with. The HiPace 80 offers high pumping speeds and maximum compression which is suitable for all gases. The Integrated drive electronics are suitable for industrial environments - Protection class IP54. Featuring its semi S2 and UL/CSA certification and laser balancing technology, the HiPace 80 is ideal for all standard applications.

Prisma Plus Spectrometer Gas Analyser

The combination of high sensitivity, maximum stability and intelligent operation make the PrismaPlus the perfect solution for mass spectrometry. Its modular design offers you a variety of application options in industrial and analytical environments, in research & development, in leak detection and semiconductor production, as well as in coating technology.

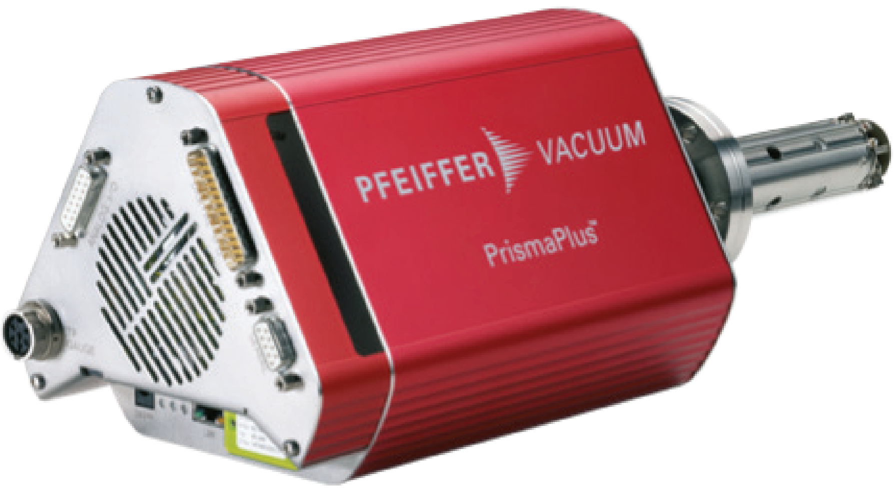
The PrismaPlus is the ideal solution for applications ranging from quality assurance and residual gas analysis right through to complex, quantitative tasks.

The Quadera® software is a further plus. In addition to being especially easy to operate, it also serves as an easy-to-read platform for transferring all measured data.

Together with a wide selection of interfaces, such as digital and analog inputs and outputs or Ethernet, integration into your system is easily achieved.

Scitek provide you with application assistance on the implementation of the PrismaPlus.

Long years of customer and application-specific experience make Pfeiffer Vacuum products your ideal partner. The added plus for gas analysis.



Multipurpose leak detectors by Pfeiffer Vacuum combine high performance and easy operation with the reliability which you have come to expect

The best in class compact multipurpose leak detectors - now with 2 years warranty

The leak detectors in our ASM 340 series guarantee top performance in vacuum or sniffing leak detection for various applications, from maintenance to applications in small production environments. These dependable leak detectors can be used both for qualitative localization of leaks as well as quantitative global or local testing. They are the only leak detectors in their class offering qualitative leak detection starting at 100 hPa before reaching the inlet test pressure.

The ASM 340 is characterized by its powerful pumping system and available in conventional or dry versions. Easy operation, ultra-fast response time and short recovery time are among the outstanding features of these compact multipurpose units. The ASM 340 is the perfect solution for everyday testing even in severe test conditions. It can be supplied with the full range of accessories, and can then be configured with either; dry diaphragm pumping units, conventional pumping units or without a backing pump unit for maximum flexibility and integration.

Highlights:

- Fastest (in its class) time to test
- High backing pump capacity for versatile use
- Rapid response time due to high helium pumping speed
- Unique capability to detect leaks starting at 100 hPa
- Impressive results in sniffing test mode, with $5 \cdot 10^{-10}$ Pa m^3/s minimum detectable leak rate for helium
- Low maintenance due to rugged design
- Detachable color control panel for enhanced ergonomics
- User friendly and customizable interface

For further information, please contact
Gino Puccini
Sales Manager
P 0427 222 080
E gino@scitek.com.au

Lastek

Photon Force Single-Photon Sensitive Cameras and Sensors

Photon Force offers a range of products and services all aimed at the acceleration of scientific and commercial research that incorporates single-photon counting and timing. Their camera range currently includes the PF32-500k as an entry-level unit, whilst the PF32-1M offers extreme speed for applications that require flexibility in readout modalities. The Photon Force PF32 cameras are the highest throughput SPAD array cameras on the market today.

- 32x32 TCSPC pixel array
- 55 picosecond resolution
- Two modes; TCSPC and photon counting
- Up to 500,000,000 photons timestamped per second

Where are Photon Force technologies used?

Photon Force products are used across a wide range of sectors to enable ultrafast, Time-Correlated Single Photon Counting with the ability to timestamp half a billion photons per second. Our cameras and sensors are primarily used in the fields of photonics, quantum optics and other scientific research to enable next generation technologies and products in a wide range of industries, spanning neuroscience, energy, communications, automotive, and beyond.

High Finesse WS8-2 High End Wavemeter

The High Finesse WS8-2 is the unsurpassed high-end instrument for wavelength measurement of pulsed or continuous laser sources. It delivers superb absolute and relative accuracy required by cutting-edge scientific research, as well as industrial and medical applications.

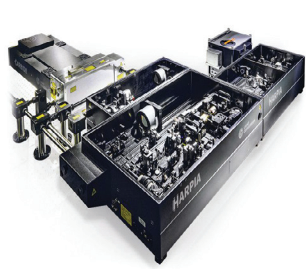
The unmatched precision of the WS8 series demonstrates the world leadership of High Finesse wavelength meters.

The photonic fiber switch at the input offers endlessly singlemode operation, making it possible to measure lasers at wavelengths across the entire spectrum with the full accuracy of the wavelength meter.

Typical Applications

The WS8-2 is the highest-end solution for wavelength monitoring and control with an absolute accuracy of 2 MHz and a wavelength deviation sensitivity of 0.2 MHz. The WS8-2 is subject to the most stringent production, testing and certification procedures and therefore offers the maximum accuracy with state-of-the-art technology.

Light Conversion HARPIA: Comprehensive Spectroscopy System



The Light Conversion HARPIA comprehensive spectroscopy system performs a variety of sophisticated time-resolved spectroscopic measurements in a compact footprint. It offers an intuitive user experience and easy day-to-day maintenance meeting the needs of today's scientific applications. Extension modules and customization options tailor the HARPIA system to specific measurement needs.

The system is built around the HARPIA-TA transient absorption spectrometer and can be expanded using time-correlated single-photon counting and fluorescence upconversion (HARPIA-TF), third beam delivery (HARPIA-TB), and microscopy (HARPIA-MM) modules. HARPIA is designed for easy switching between measurement modes and comes with dedicated data acquisition and analysis software. Each module is contained in a monolithic aluminium body ensuring excellent optical stability and minimal optical path lengths. For a single-supplier solution, the HARPIA spectroscopy system is combined with a PHAROS or a CARBIDE laser together with ORPHEUS series OPAs. HARPIA also supports Ti:sapphire lasers with TOPAS series OPAs.

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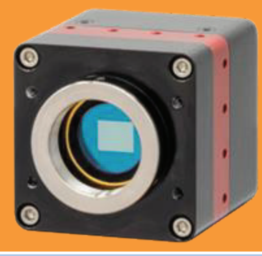
Raptor Photonics

A leading developer and supplier of next generation, high-performance digital camera solutions for the Scientific, Surveillance and Aerospace markets. Raptor offers a range of CCD, EMCCD and InGaAs (SWIR) solutions. As well as standard products, Raptor provides custom solutions to OEM and Instrumentation companies around the World



Tucsen Photonics

Camera Technology Focussed on Scientific and Challenging Inspection

- Tucsen a global company designing and manufacturing in China
- Consistently Delivering Value

Dhyana 400BSI V3 – Not Just a Product Line Extension but a Best Engineers Camera

Photon Force

PF32 - Time-Correlated Single-Photon Counting Camera at 55 ps time resolution.

In-pixel time-tagging for time-resolved imaging and photon counting

NIT

Thermal Imaging Cameras

NIT New Infrared Technologies

The thermal camera LIR320, with its compact dimensions, industrial connectivity and capabilities oriented to 4.0 Industry.

Vigo Photonics

VIGO PHOTONICS

Vigo Photonics has developed a unique technology for manufacturing instruments for quick and convenient detection of 1 – 16µm infrared radiation. The instruments operate in ambient temperature or are cooled with simple and inexpensive thermoelectric coolers.