School of Chemistry and Physics of QUT

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INTRODUCTION

Queensland University of Technology:
QUT is a major Australian university with a global reputation and a 'real world' focus. Our courses equip our students and graduates with the skills they need for the world of today and tomorrow.

QUT is an ambitious institution, with a rapidly growing research output focused on technology and innovation. The Times Higher Education 2020 ranked QUT in the top 180 universities in the world and the best young university in Australia.

In 2019, QUT released its new strategic plan, Blueprint 6, with the aim to be 'the university for the real world', and to provide transformative education and research relevant to its communities.

With more than 50,000 students, QUT places a premium on the national and international accreditation of our professional degrees. QUT is transforming the learning experience and embeding work integrated learning in courses, and has a strong focus on developing entrepreneurial skills.

The international award-winning Science and Engineering Centre at Gardens Point campus is home to The Cube, one of the world's largest digital interactive learning and display spaces, and headquarters of the Institute for Future Environments.

QUT is well known for its strong links to industry and government and the high impact of its research with multidisciplinary teams of researchers working to solve real-world problems.

QUT has been named one of the fastest rising universities in the world, and top in Australia, for scientific research in the 2019's Nature Index of high-quality research outputs.

Fig. 1: Aerial view of QUT.

School of Chemistry and Physics:
The School of Chemistry and Physics [1] was formed in January 2020 and comprises approximately 70 academic staff, including 2 Australian Research Council (ARC) Laureate Fellows, 5 ARC Future Fellows, 6 ARC DECRA Fellows, 3 ARC College of Experts members, and over 120 Higher Degree by Research (HDR) students. The School conducts research in diverse areas, earning the ARC's highest rankings of 5 (well above world standard) in Condensed Matter Physics, Other Physical Sciences, Macromolecular and Materials Chemistry, Organic

Chemistry, Theoretical and Computational Chemistry, Materials Engineering, and Nanotechnology. The cutting-edge research undertaken in the School is well integrated with QUT's flagship research centres such as the Centre for Materials Science and the Centre for Clean Energy Technologies and Practices. Researchers and students in the school benefit from the easy access to the Central Analytical Research Facility (CARF), located within QUT's $230M Science and Engineering precinct, that houses state of the art analytical equipment.

The School offers teaching programs in the Chemistry and Physics majors in the Bachelor of Science, complemented by a range of minor options in Analytical Chemistry, Astrophysics, Forensic Science, and Nanotechnology. The undergraduate degrees are all accredited by the Australian Institute of Physics and the Royal Australian Chemical Institute, depending on the study areas. The School also offers a Master of Medical Physics course, the first of its kind in Australia, accredited by the Australasian College of Physical Sciences and Engineers in Medicine.

RESEARCH ACTIVITIES

Surface Science and Nanomaterials

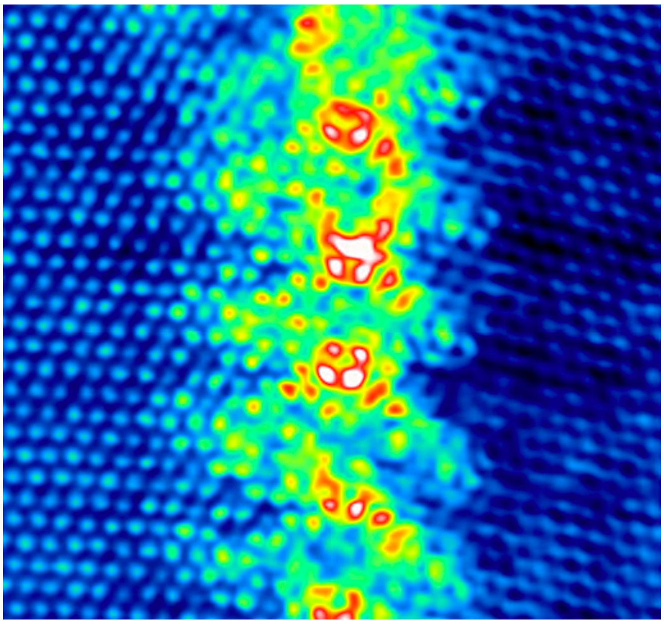

Fig. 2: Graphene ripples generated by grain boundaries in highly ordered pyrolytic graphite visualised by STM.

The Surface Science and 2D Materials Group [2] undertake research focusing on creating, understanding, and controlling at molecular-scale the surfaces and interfaces of functional materials and low-dimensional materials for applications in emerging electronics, energy, environmental and sensing technologies. A significant research focus has been devoted to the study of the growth and synthesis of 2D materials, including graphene and transition metal dichalcogenides, as well as polymers and covalent organic frameworks with bottom-up approaches where the delicate balance of kinetics and thermodynamics of atoms and molecules are precisely controlled to form nanoscale architectures at surfaces. Innovative surface and interface engineering approaches have been developed to tailor the electronic, piezoelectric and optoelectronic properties of emerging electronic materials, such as diamond and graphene, enabling next-generation electronics, carbon-based supercapacitors and ultrasensitive gas sensors. The group builds research capacity in surface science by leveraging on the state-of-the art surface science instrumentation hosted by CARF, including the first scanning tunneling microscope (STM) in Queensland, as well as the synchrotron facilities both in Australia and around the globe; it also develops new instrumentation capability in low-energy inverse photoelectron spectroscopy allowing a comprehensive characterisation of the electronic structures of new materials.

The Inorganic Nanomaterials Lab [3], led by ARC Laureate Fellow Prof. Dmitri Golberg, pioneers design, synthesis and characterisation of inorganic nanomaterials for structural and green energy applications. The scope of research interest ranges from carbon, boron nitride and dichalcogenide nanotubes and nanosheets, to various prospective 0D, 1D and 2D phases, such as metallic nanoparticles and nanowires, MXenes, borophenes etc. Underpinning these research activities is the development and implementation of spatially-resolved dynamic in-situ transmission electron microscopy (TEM) that allows the measurement of a nanostructure response to mechanical, electrical, optical and thermal, and other external stimuli under operando conditions. The team is instrumental to the establishment of a new $4.7M double-aberration corrected super-high resolution TEM (JEOL-NEOARM) with in situ capabilities which is the only microscope of its kind in Australia.

The School also conducts world-leading research dedicated to developing smart multifunctional metal oxide nanomaterials by learning from nature for applications in sustainable energy and environmental technologies, including next-generation energy conversion and storage devices, green fuel generations, and sustainable environmental remediations. Novel bio-inspired interfaces and surfaces with novel multiple functionalities have been developed based on understanding the relationships among the composition, structures, and properties of biological surfaces by a combinations of modern analytical technologies and theoretical calculations.

Medical Physics

Medical physics research at QUT covers the specialty areas of radiation oncology, diagnostic imaging and radiation protection. University academics collaborate closely with multi-disciplinary clinical teams on contemporary problems in modern healthcare.

In radiation oncology, research is being performed into the use of electronic portal imaging devices (EPIDs) for in-vivo dosimetry, addressing one of the significant challenges in the delivery of precise and personalised radiotherapy treatments. This work has involved experimental and Monte-Carlo modelling of the radiation beam interactions in the medical linear accelerator, patient, and EPIDs. Novel radiation therapy approaches are being developed in animal preclinical models with their synergistic effects in combination with immunotherapy. This also includes research on the development of adaptive strategies to correct in real time treatments when the patients' conditions change (due for example to internal organ movements), and using automatic organ contouring approaches to spare critical structures from unnecessary radiation dose delivery, or to evaluate quantitatively the systematic planning variations among different clinical centres.

Magnetic Resonance Imaging (MRI) research at the School is focused on applications of quantitative MRI to biological tissues and models of disease. Quantitative characteristics measured using MRI include, among others, spin-relaxation rate constants and the diffusion tensor. Both of these are closely related to the composition, organisation and microstructure of the tissue, and can therefore be used for tissue characterisation. Recent research in this area has included applications of quantitative spin-relaxation imaging to study the biomechanics of articular cartilage as well as the progression of Post-Traumatic Osteoarthritis in murine models; applications of quantitative diffusion imaging to study the biomechanics of articular cartilage and spinal intervertebral disc; and diffusion-based characterisation of murine models of cancer. Research in advanced quantitative medical imaging is investigating how to use ultrasound as a real time volumetric mapping tool of human tissues, to guide in a reliable and accurate way complex medical procedures. Several novel methods which make use of cutting-edge artificial intelligence technology are being developed to show where the treatment target and the organs at risk are at all times during treatments in radiation therapy, or to inform robots during autonomous minimally invasive surgery so they can perform safe and effective procedures.

Photophysics and Photochemistry

The School conducts frontier research looking into not only the fundamental interaction between light and matter but also exploiting the interaction for transformative materials research. Exciting projects of the Nanosensors & Molecular Diagnostics Group [4] focus on building a multi-disciplinary platform for fast, accurate and non-contact detection and quantification of chemical and biological analytes. This is enabled by the development of innovative Raman spectrometry techniques and methodologies for analytical and bio-analytical applications in health, forensics, toxicology, and homeland security. This attracts partnership with the Australian Federal Police to create a drug sensing platform, and with the global leader in the Defence Industry, EPE, to create a handheld Raman sensing platform.

The Soft Matter Materials Laboratory [5], led by ARC Laureate Fellow Prof. Christopher Barner-Kowollik (also the Deputy Vice Chancellor Research & Innovation and Vice President of QUT), pioneers fundamentally new approaches in synthesis that exploits the selectivity and efficiency of light. Avoiding the usually required harmful UV light in light fuelled reaction processes, new polymerization and ligation techniques that make use of benign visible light are being developed. Exceeding the spatio-temporal control of light allows the determination of when and where a reaction takes place by designing chemical reactions that also respond selectively to the colour of light. Such wavelength-gated systems enable molecular surgery by altering specific parts of molecules while leaving others untouched – and on the materials level even enable the fabrication of multiple materials from only one photoresist as the function of the colour of light. Polymers that can be made and unmade again in the presence of a certain stimulus are being developed to address the global problem of lifetime cycles of plastics. Exploiting chemical bonds that are only stable in the presence of light and autonomously disintegrate in the dark provides a means for control of the lifetime of synthetic materials. In combination with ring-opening polymerization (ROP) or reversible deactivation radical polymerization techniques such as atom transfer radical polymerization (ATRP) or reversible addition-fragmentation chain transfer (RAFT) polymerization, light-induced tools provide the opportunity for the rapid design of complex macromolecules under ambient reaction conditions. Light triggered ligation protocols enable applications in hybrid material design, most notably for spatially resolved (bio)surface design and in lithographic applications such as 3D laser lithography.

Pioneering contributions to photosynthesis and photocatalysis include the use of photons and plasmonic metal nanoparticles to control the outcome of chemical reactions that are difficult to execute using thermal energy, plasmonic electromagnetic field based molecule capture, and metal-free graphitic carbon nitride photocatalysis for visible-light induced synthesis and conversion. These innovations drive the development of catalysts with maximized utilization efficiency of plasmonic metals, the design of materials and processes for selective conversion of hydrocarbons, and biomass-based feedstocks into higher valued products. Molecular level insights into the underlying mechanism that underpins light-controlled catalytic reactions are utilized to guide the synthesis of catalysts with targeted geometries, compositions and architectures.

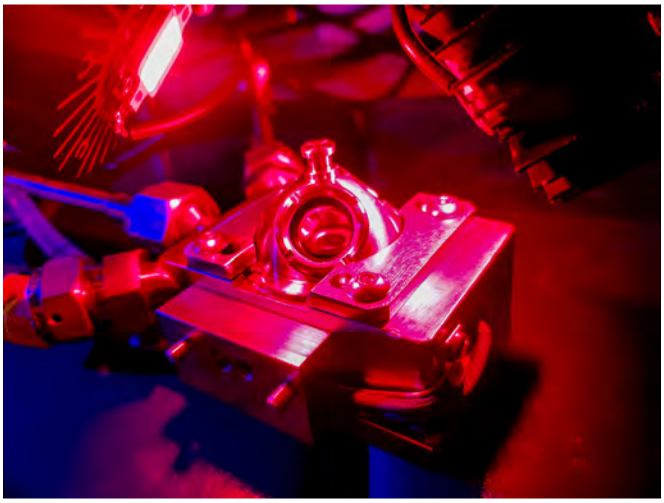

Fig. 3: Researchers at QUT use light to drive molecular reactions.

Computations and Modelling

Over the last 10 years, new theory, algorithms and powerful hardware have driven massive advances in high performance computing to enable an unprecedented acceleration in the discovery of new materials for applications in energy, environment, and nanoelectronics. Research in the Computation and Modelling group at QUT is focused on discovering new low dimensional nanomaterials using high throughput computational screening. The exploration of electronic functionality and how it varies with novel molecular architecture runs ahead of experimental synthesis yet provides insights into the types of structures that may prove profitable for targeted experimental synthesis and characterization. Some predicted materials at QUT have been successfully synthesized in experiments.

Materials' properties are in principle determined by electronic structure. Tunning electronic structure via engineering the impurities, surfaces, interfaces, and dimensions of materials has been another focus of research at QUT. By shedding light "from the bottom up", state-of-the-art first-principles computation can offer molecular-level understanding of novel physics and chemistry in low dimensional nanomaterials and suggest what types of structures could prove useful for achieving targeted properties.

Nanoscale materials are difficult to manipulate and characterize in experiments because of their small size, which raises the conundrum of how to expedite the exploration and targeted design of new materials. Through engaging with leading experimental groups worldwide, theoretical research at QUT has provided a powerful complement to experimental synthesis and characterization. The collaborations have led to many important discoveries in particular in the fields of novel energy materials and battery materials.

Plasma Physics and Chemistry

Low temperature plasma nanofabrication is a versatile technology for energy conversion, storage and utilization. Plasma processes are used for materials synthesis and processing, in particular for the production of devices and systems for applications in the areas of energy conversion, storage and utilization. As such, plasma physics and chemistry is a rapidly advancing enabling research area. The plasmas feature uniquely non-equilibrium reactive medium which is suitable for advanced nanoscale synthesis and processing. This feature is related to the high reactivity of the plasma empowered by highly-energetic electrons and diverse reactive species such as ions, excited molecules and radicals. Plasma methods have been used for the nanoscale control of energy and matter leading to the production of a broad range of nanostructures such as graphene sheets of various orientations, other two-dimensional materials, nanowires, quantum dots and small nanoparticles and others.

Energy Materials and Devices

The study of materials that are applicable in energy devices has gained significant momentum in the last decade. QUT is engaged in the synthesis, characterisation and testing of new and advanced materials in areas such as electrochemical water splitting to produce green hydrogen, Li-ion batteries, beyond Li-ion battery technology, supercapacitors and solar cells. This encompasses the replacement of precious metal catalysts with cheaper alternatives that have enhanced performance for water splitting, improving anode and cathode materials for Li-ion batteries, developing alternative battery technologies such as Al, Mg, K and Na ion batteries, producing new materials for supercapacitors and synthesising robust high performance materials for perovskite solar cells. A key aspect of energy materials research at QUT is transferring the fundamental understanding and outcomes developed at the bench scale to pilot plant level and the fabrication of commercial prototypes. This is reflected in QUT's pilot battery manufacturing plant at Banyo and the Redlands Renewable Energy Facility which integrates different types of solar cell technologies with electrolysers, batteries, and fuel cells into a micro grid with plug and play opportunities for new technologies. Both fundamental and applied work in energy materials is supported through ARC Industry Hubs, the Future Batteries Industries Cooperative Research Centre (CRC), the Future Energy Exports CRC and the Australian Renewable Energy Agency.

Organic Electronics

Organic /printed electronics is a field of materials science pertaining to the design, synthesis, characterization, and application of functional semiconductors such as organic (small molecules, dendrimers, polymers), inorganic (metal oxides, 2D materials, quantum dots) or hybrid (organic-inorganic composite) that exhibits desirable optoelectronic properties. These next generation materials can be used for flexible and printed electronics since they offer easy solution processability and can be deposited on various substrates from conventional rigid, flexible plastic to the stretchable rubber substrates.

At QUT, the organic and printed electronic research group focuses on the development of various new advanced functional materials for the next generation optoelectronic devices. Such optoelectronic devices can be classified based on their applications for display, sensing, environmental and health monitoring, smart living, wearable electronics, robotics, bioelectronics, Internet of things (IoT) and energy efficient technologies. The group also leads the creation of new components such as organic light emitting diodes (OLEDs), thin film transistors (TFTs), photovoltaic devices (PV), photodetectors, chemical/bio sensors, artificial muscles, battery electrodes, supercapacitors, and other devices where an active semiconductor/conductor plays a significant role. Some of the recently highlighted high impact research includes the development of fluorescent carbon dots from human hair waste. These quantum dots were successfully used as an active light emitting layer together with a polymer matrix for the fabrication of flexible display devices. This research work was published in Advanced Materials and Wiley has highlighted a video on this work [6].

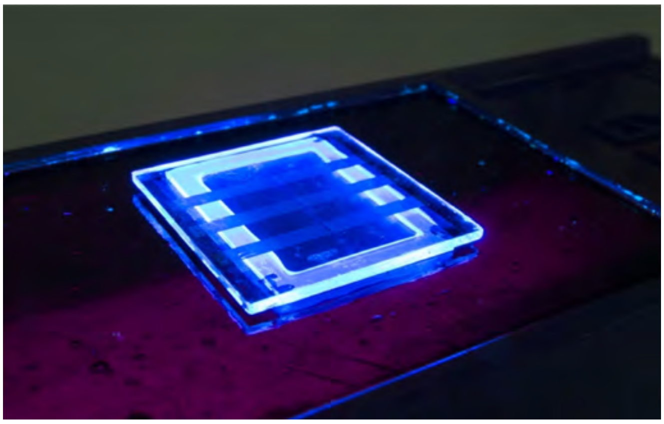

Fig. 4: Light emitting devices made from carbon quantum dots derived from human hair waste.

Molecular Science

Current research in molecular science lies at the core of the School's mission, from the synthesis of functional molecules (organic, organometallic and coordination compounds) for use as sensors, switches, emissive components of OLEDs, profluorescent sensors, supramolecular cages, capsules, rotaxanes and catenanes to polymer precursors for creation of functional macromolecular materials. QUT is equipped with state-of-the-art laboratories and supported by access to the full suite of analytical instrumentation for product characterisation. Some current highlights are described below.

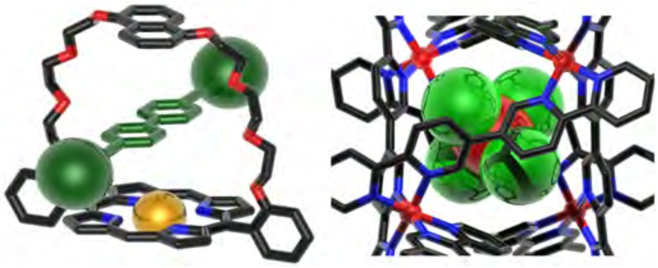

Fig. 5: The unique space within heterosupramolecular cages and capsules can be exploited for applications requiring selective encapsulation including anion sensing and chromatographic separation.

The unique topologies of catenanes and rotaxanes have found application in areas such as sensing, catalysis, drug delivery and even form the basis of molecular machines. Current research focusses on the development of methodologies for the synthesis of mechanically interlocked architectures in solution and on solid supports for potential applications to sensing and switching. Exciting new projects focus on how advanced mass spectrometry techniques can be used in the gas-phase synthesis and characterisation of interlocked complexes, including ephemeral radical-containing species that are difficult to isolate and characterise in solution.

Pioneering contributions to free radical chemistry include the use of nitroxides to study biological systems, polymer degradation and environmental pollution. Contributions include the development of anti-fouling and anti-inflammatory materials and coatings that utilise nitroxides for applications ranging from biomedical implants to chronic wounds and the design and development of fluorescent probes to study radical formation in a range of applications including materials degradation and in diseases involving oxidative stress.

Molecular crystals have long been thought to be brittle and inelastic and as such their unique properties were assumed to be inaccessible for applications requiring mechanical flexibility. A recently discovered suite of crystals containing metal complexes are so flexible they can be reversibly tied in knots. The development of a method for determining the molecular mechanism of elastic deformation in molecular crystals means it is now possible to design and prepare a wide range of flexible crystals with tunable magnetic and optical properties for potential applications in flexible devices.

In other research, controlled radical polymerisation techniques are used to design and prepare new polymer materials to solve clinical challenges. This includes responsive polymers, branched polymers and self-assembled systems to develop materials that can be used as coatings to prevent bacterial fouling, visualise the development of disease or aid in the treatment of cancer by radiotherapy. Inspired by nature's functional macromolecules such as enzymes, synthetic avenues to generating functional 3D architectures from synthetic polymer chains, so called single chain nanoparticles, are also being developed.

Fig. 6: QUT's Centre for Materials Science drives cutting-edge research in materials innovation.

Centre for Materials Science

The Centre for Materials Science is QUT's fundamental scientific engine room for building and developing critical mass in materials science to achieve high-quality and high-impact research that is nationally and internationally leading [7]. The Centre, co-led by Prof. Kathryn Fairfull-Smith and ARC Laureate Fellow Prof. Dmitri Golberg, fuses cross-disciplinary fundamental research expertise within QUT, enabling a coherent research space to undertake curiosity-driven materials discoveries. With its assembled critical mass of high-calibre researchers in materials science, the Centre provides innovative high-quality and high-impact materials solutions by discovering and creating new materials, analysing their properties and functions at atomistic and molecular level, implementing them into existing and emerging technologies (e.g., quantum computing, topological insulators, catalysis, flexible optoelectronics, clean energy production and storage) as well as transferring this knowledge to the Real World in a human-centred society that balances economic advancement with the resolution of societal problems.

The Centre also strives to provide an intellectually stimulating collaborative environment that nurtures emerging research talent from the PhD level to the Early Career Researcher (ECR) level, while it provides research space and freedom to the leaders in their field. It achieves this by providing mechanisms to support the research activities of all Centre members and celebrate and promote Centre achievements in a positive collaborative culture. The Centre places special focus on supporting the research opportunities of ECRs by providing research and travel bursaries, mentoring and HDR supervision support.

The Centre has four core Research Themes:

Soft matter materials theme encompasses the discovery and development of synthetic strategies from small molecule systems to complex macromolecular constructs that are able to execute specific functions controlled by external fields such as light. This theme develops advanced soft matter functional materials that solve key technological challenges in real world applications.

Hard condensed matter materials theme fuses QUT's strength in 0D, 1D, 2D and 3D nanostructures as well as their synthesis and characterization, by exploring atomic structures, their crystallography and spatially-resolved chemistry at the world-highest levels of spatial, temporal and energy resolutions. This theme works to create a full bank of condensed matter 0D, 1D, 2D and 3D materials with on-demand electrical, mechanical, optical, thermal and magnetic properties for reliable practical, real world applications.

Computation, prediction and modelling theme employs state-of-the-art computational facilities to accurately predict meta-material properties to direct the synthetic themes. This Research Theme accelerates the discovery of novel hard and soft materials through the prediction of new materials and in-depth understanding of materials' structure-property relationships.

Materials characterisation theme develops and deploys advanced technologies directed towards the frontiers of mixture analysis and light-matter interactions. This theme solidly establishes QUT's reputation at the forefront of analytical measurement and technique development, both nationally and globally, by prioritising the use of novel techniques that capitalise on our strategy of bringing together cutting-edge instrumentation and world-class technical expertise.

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Jennifer MacLeod is an Associate Professor and Head of School of Chemistry and Physics at Queensland University of Technology (QUT). After receiving MSc and PhD degrees in Physics from Queen's University (Canada), she went on to hold postdoctoral positions at the Institut national de la recherche scientifique (Canada) and the Università degli studi di Trieste (Italy) before joining QUT in 2015. Her research is in surface science, with a particular focus on instrument development and spectroscopy and microscopy of molecular systems.