Abstracts are provided by presenters.

1. Sedimentology and characterisation of marginal reservoir facies in fluvial and delta top depositional systems

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Sandstones deposited in delta plain settings are significant petroleum reservoirs around the World. These sandstones create important but complicated reservoirs which include channel deposits and adjacent crevasse splays. The role of the channel sandstones as reservoirs is well documented but the importance of the crevasse splay deposits is less understood, especially in “tight gas” settings. The current research aims to improve understanding of crevasse splay sandstones from a reservoir perspective providing their composition, architecture, connectivity, a new classification scheme, controlling factors and reservoir quality by studying modern (Google Earth data) and ancient (LiDAR & UAV data) analogue delta top settings.

2. A Bounce as a beginning?

Chandrima Ganguly
University of Cambridge

I will describe an alternative theory describing the early universe, that of cyclic cosmologies. I will discuss the basic mechanism of how it hopes to resolve the isotropy problem, and then will present criticisms of the mechanism. I will show that such models are unsuccessful in achieving isotropy in their current incarnation.

3. Aharonov-Bohm effect in Bose-Einstein condensates

Tobias Haug
National University of Singapore

Atomtronics is an emerging field in quantum technology to realize circuits of any shape with atoms cooled down to very low temperatures. We use this platform to investigate the Aharonov-Bohm effect. It changes the current of particles enclosing a magnetic field depending on the field strength. This is the case even when the particles do not interact with the magnetic field directly. The time dynamics and the effect of scattering is not well understood. In an atomtronic setup, we find that for strongly interacting Bosons the Aharonov-Bohm effect vanishes and we suggest various applications for the system.
4. Low-energy electron-molecule collision studies using velocity map imaging spectrometer

Pamir Nag
Indian Institute of Science Education and Research Kolkata

Low-energy electron-molecule collision leading to dissociative electron attachment (DEA) is an important process from the fundamental as well as the application point of view. DEA is a two-step resonant process resulting into a final anionic and neutral fragments from a parent neutral molecule via intermediate temporary negative ion (TNI) state. DEA study of molecules are important starting from electrical discharges, atmospheric chemistry, installer medium chemistry to radiation induced damage of living cell and biologically important molecules. We have developed a velocity map imaging spectrometer to study the kinematically complete information of the dissociation process and applied the same to study different molecules.

5. Towards understanding a mechanism of fungal virulence

Natalie C. Bamford¹,², Brendan D. Snarr³, Fabrice N. Gravelat³, François Le Mauff³, Mark J. Lee³, Donald Sheppard³, P. Lynne Howell¹,²

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Aspergillus fumigatus (AF) is the second most common cause of hospital related fungal infections. AF can grow as multicellular communities called biofilms. Galactosaminogalactan (GAG) is an exopolysaccharide required for AF biofilm formation and a key virulence factor. Deletion of the gene sph3 results in no biofilm or GAG production. We conducted structural and functional assays on Sph3 and found it to be a novel polysaccharide cleaving enzyme. Addition of purified Sph3 to AF cultures leads to biofilm disruption and release of GAG oligomers. This work furthers our understanding of biological mechanisms and fungal virulence.

6. Advanced glycation end products (AGEs) and diabetic complications

Mohammed Jainuddin Yousuf Viswa Sheik
MedAll Health Care (P) Ltd, India

During long standing hyperglycemic state in diabetes mellitus, glucose forms covalent adducts with the plasma proteins through a non-enzymatic process known as glycation. The non-enzymatic reaction between the free amino groups of proteins and carbonyl groups of reducing sugars is known as Maillard reaction. This reaction is subdivided into three main stages: early, intermediate and late. In the late stage of glycation, irreversible compounds called advanced glycation end products (AGEs) are formed. The formation of AGEs plays an important role in diabetic complications like retinopathy, nephropathy, neuropathy, cardiomyopathy and aging. The outcomes of the study will be discussed in detail.
7. An optimized workflow for the identification of heparin-binding cysteine-rich peptides from plant origins

Shining Loo, Antony Kam and James P Tam

Nanyang Technological University

Heparin belongs to the family of glycosaminoglycan. Many heparin-binding peptides are known to be growth factors, coagulation factors, DNA-binding proteins, protein synthesis factors and lipoproteins. Hence, our laboratory is interested to develop an optimized workflow for fast identification of heparin-binding cysteine-rich peptides (CRPs) from plant extracts. Briefly, the proposed pipeline consists of fractionation using heparin affinity column followed by an in-house high throughput peptidomic sequencing technique. Here, using the extract of *Pereskia bleo*, we present this optimized methodology which led to the discovery of a novel heparin-binding CRP.

Acknowledgement

This project was supported in part by the National Research Foundation (NRF-CRP8-2011-05) of the Prime Minister’s Office of Singapore.

References


8. Investigating the resistance to targeted therapy in triple-negative breast cancer

Nuramalina Mumin

University of Oxford

Triple-negative breast cancer (TNBC), which accounts for about 10% of all breast cancer cases, is a highly aggressive breast cancer and challenging to treat due to the absence of approved targeted therapies. HSP90 inhibitors have shown promising anti-cancer activities. However, TNBC can develop resistance to these inhibitors. In order to investigate the underlying mechanisms of resistance, we utilised a 96-well based screen with a bioactive small molecule library and gene expression profiling (RNA-Sequencing). A greater understanding on the effects of targeted therapies might help in developing effective therapeutic strategies and identifying novel drug combinations for TNBC.

9. Competition between a protein and a small RNA dictates the regulation of the Opp transporter in *Escherichia coli*

Marie-Claude Carrier

Université de Sherbrooke

Bacterial small RNAs (sRNAs) are powerful regulators of gene expression and play essential roles in maintaining cell homeostasis. sRNAs can be assisted by protein chaperones such as Hfq to facilitate target regulation. We focused our attention on exposing the complex network of MicF sRNA, an
effector of the osmotic shock response. We identified a new target of MicF, the \textit{oppA} mRNA. \textit{OppA} is part of the oligopeptide transporter \textit{Opp}. Short bactericide peptides are imported through the \textit{Opp} transporter. We propose a completely new sRNA-dependent mechanism of action based on the competition between the Hfq chaperone protein and MicF sRNA.

\textbf{10. Ionophoric effects of the antitubercular drug bedaquiline}

Kiel Hards

University of Otago

Antibiotics generally target one of five major bacterial targets or pathways, which are becoming limited due to increasing drug resistance. Bedaquiline, a new FDA-approved antitubercular, targets energy metabolism and so defines it as the sixth target for antibiotics. This is a relatively unexplored target-space, as bedaquiline has only been FDA-approved for 5 years. Much remains unknown about the molecular effects of bedaquiline, limiting the development of second-generation compounds. In this work, we determine that bedaquiline has the ability to disrupt pH and potassium homeostasis, a previously unreported effect. These results can direct drug-development in this space.

\textbf{11. Amino acid surfactants - A promising alternative to conventional surfactants in cosmetics and soap formulations}

Nausheen Joondan

University of Mauritius

Amino acid based surfactants are considered to be a safer alternative compared to conventional surfactants due to their biodegradability and low toxicity. This study involves the synthesis, physicochemical properties and biological activities of novel aromatic and cyclic amino acid surfactants. These surfactants possess good antibacterial activity. Their mode of action has been established by investigating their interactions with phospholipid vesicles. Their antibacterial effectiveness and foaming abilities in mixed surfactant systems (amino acid based surfactants-conventional surfactants mixtures) together with a lower ocular irritation and toxicity profile enable them to be promising candidates to be used in cosmetics and detergent industry.

\textbf{12. Structural Determinants of Membrane Fission}

Srishti Dar

Indian Institute of Science Education and Research Pune

Membrane fission is fundamental to diverse cellular processes such as vesicular transport, synaptic transmission, organelle biogenesis and cell division. Biochemical screens for effectors of membrane fission and a mechanistic analysis of this process requires a tubular membrane template as a substrate. Alternately, I have developed a facile assay system of arrayed supported membrane tubes (SMrT), where the membrane tube dimensions can be controlled to mimic the topology of tubular intermediates generated during fission (Dar et al., Nat Protocols 2017)). Using this assay, which allows visualization of hundreds of single membrane fission events in real-time, I can now trace the
The evolution of membrane intermediates to nanometer precision. These results published recently unambiguously establish 1) a role for GTP hydrolysis in bringing about membrane constriction leading to a successful fission event (Dar et al., Nat Cell Biol. 2015); and 2) the catalytic role of the membrane binding pleckstrin-homology domain (PHD) in contributing to faster kinetics of the fission reaction (Dar et al., Mol Biol Cell 2017). My current research is focused on adapting our assay system to mimic the cylindrical topology of intermediates generated prior to cytokinesis. By reconstituting the cytokinetic ring in the lumen, I hope to understand the mechanisms by which proteins involved in cytokinesis manage membrane remodelling during cell division. In sum, my research has contributed both to technology development to monitor membrane-remodeling events and critical re-evaluation of dynamin function that substantially improves our understanding of the important process of membrane fission.

13. A sharp interface model and its numerical approximation of solid-state dewetting in three dimensions

Zhao Quan

National University of Singapore

Solid thin films on the substrate are typically unstable and can exhibit complicated morphologies evolution even below their melting temperature. Driven by capillary instabilities, the thin film can produce a series of growing holes, retracting edges, or even break up into small islands. This process, known as dewetting, tends to minimize the total surface energies of the system via surface diffusion while preserving the volume of the thin film. So based on the thermodynamic variation, we derive the sharp interface model of solid-state dewetting on a flat substrate. The governing equations for the problem belong to the 4-th order geometric partial differential equations which include the surface diffusion flow and contact line migrations. We then propose a variational formulation for the sharp interface model and apply parametric finite element method to solve it.

14. Metal-free catalysis: Toward a greener chemistry

Etienne Rochette

Université Laval

The detrimental impacts of the chemical industry on the environment are undeniable. Yet it is also one of the industry that as improved the most our quality of life. Catalysts are at the core of the development of safe, inexpensive, sustainable and green chemical processes, but are often based on transition metals that can be expensive and toxic. In our research, we try to demonstrate that with careful catalyst design, atoms that are thought less reactive such as the main group elements, can achieve surprising reactivity and allows us to develop a greener chemistry.
15. A piperazine-based library for fragment-based lead discovery

Errol Samuel

Baylor College of Medicine

Drug-like molecules can be considered as a combination of smaller binding fragments. Screening for these fragments, then expanding or linking them is called fragment-based drug discovery (FBDD), an approach now recognized as a powerful way to create high-quality drug-like molecules in the quest for new therapeutics. However, the vast majority of fragment screening collections are comprised of 2-dimensional molecules, limiting their coverage of chemical space and their potential of binding diverse biological targets. My research involves the synthesis and screening of novel and diverse 3-dimensional fragment libraries, with the goal of improving chemical space coverage and consequently, chances for success.

16. Synthesis of high silica porous material from waste coal fly ash

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Coal fly ash is a waste material produced during the combustion of coal for electricity generation. The advantage of this material is based on the elemental composition which is majorly silica and aluminium. Nanocrystal beta-zeolite was prepared through the hydrothermal synthesis of fly ash based extracted alumina-silica. The octahedral morphology and the well-defined spectra with two significant peaks at 7.7° and 22.7° 2θ of the product is similar to a distinctive beta zeolite topology. The achieved high surface area 609.41 m²/g of the obtained crystals is an indication that the fly ash based beta zeolite will be suitable for different catalytic applications.

17. Designing solvent systems for improved organic solar cell stability

Sarah Holliday

University of Washington

Organic solar cells are one emerging technology that has the potential to substantially reduce the cost of solar energy production due to the use of earth-abundant materials and compatibility with high throughput, roll-to-roll printing techniques. A large amount of research has focused on increasing the efficiency of these devices by developing new organic polymers, leading to efficiencies that are now competitive with amorphous silicon. However, the lifetime of these organic solar cells is much shorter due, in part, to photooxidation of the polymer. Here we discuss the factors contributing to this degradation, including the use of high boiling point solvent additives that can remain in the film after
fabrication and facilitate the diffusion of oxygen into the film. A new solvent system is proposed that offers both high efficiency and greatly enhanced stability relative to the traditional solvent systems.

18. Application of transition metal sulfides as cathode materials in all-solid-state lithium batteries
Jean Pierre Mwizerwa
Ningbo Institute of Material Technology and Engineering

Due to the increasing need of hybrid electric vehicles (HEVs) and portable electronic devices, the demand for high safety, energy and environmental friendliness rechargeable batteries as energy storage systems has become the most viable option. As the most dominant power sources for electrical energy-storage LIBs cannot satisfy the demand of fast-growing market from small portable devices to large-scale electric vehicles not only due to their limited practical energy density but also their safety issues. All-solid-state lithium batteries which are stable and safe are considered as novel candidates for HEV and EV power sources. In this regard, the naturally abundant, inexpensive and environmentally benign transition metal sulfides are considered as larger capacity, high safety cathode materials for ASSLBs for the next generation of rechargeable batteries over transitional cathode materials.

19. Ionic liquids and their binary systems with water in organic synthesis
Gulshan Ara
University of Dhaka

Ionic liquids (ILs), composed exclusively of ions, and their binary mixtures with water have been one of the most promising materials in green chemistry due *inter alia* to negligible vapor pressure. The nature and strength of intermolecular forces in ILs have been investigated in detail. The prospect of the ILs and its binary mixtures with water at varying compositions as catalyst and reaction medium for Michael addition reaction was investigated. The properties have been correlated with the structure of the ILs and the composition to understand the role of the ILs in the reaction mechanism at the molecular level.

20. Supercritical CO2 as a green alternative of organic solvents for monolayer grafting
Bhavesh Bhartia, Sreenivasa Reddy Puniredd*, Cedric Toradec*, Madapusi P. Srinivasan*
National University of Singapore

Organic molecular functionalization offers the ability to precisely control and modulate the surface properties which is becoming increasingly important with constant decrease in device size. However, the current organic solvent based methods not only restrict the potential advantage of surface functionalization but are also environmentally damaging. Our work is focused on establishing supercritical CO2 (SCCO2) as a carrier fluid and processing medium for monolayer grafting. The advantageous and unique physical properties of SCCO2 not only allows the improvement in quality of
already present monolayer systems but also permits the deposition of novel monolayer systems which cannot be deposited using organic solvent based methods.


Chia Xinyi

Nanyang Technological University

Our primary source of energy has been derived from non-renewable fossil fuels that leave behind a large carbon footprint. Relentless efforts have been channelled into developing technologies for clean and sustainable energy. A popular option since long ago is the water-splitting method to produce hydrogen gas (H\textsubsc{2}) as a clean energy carrier. Recently, the limelight is on economical layered catalysts, in particular, transition metal dichalcogenides (TMDs); that effectively reduces the thermodynamic barrier during the process. Here, we explore the prospect of electrochemical strategy via a reduction or oxidation towards improving the catalytic properties of layered TMD materials for hydrogen evolution.

22. Synthetic studies towards an enantiomeric pair of indole alkaloids isolated from the roots of \textit{Isatis indigotica}

Emma K. Davison* and Jonathan Sperry

University of Auckland

The unnamed enantiomeric pair of indole alkaloids 1a and 1b were isolated from the roots of the herbaceous plant \textit{Isatis indigotica} which is commonly used in Chinese traditional medicine. These natural products contain a dihydrothiopyran and a 1,2,4-thiadiazole heterocycle, the latter being an exceptionally rare motif in Nature. Synthetic studies towards 1a and 1b will be discussed, whereby a late-stage intermolecular Heck reaction between 2 and 3 is proposed to construct the complete heteroaromatic framework of the natural products.

23. Microemulsions as a Template to Control Stability and Aggregation of Silver Nanoparticles

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Institute of Glass & Ceramic Research and Testing (IGCRT)
Bangladesh Council of Scientific and Industrial Research (BCSIR), Dhaka, Bangladesh

Silver nanoparticles (AgNPs) with tunable properties have been a fascinating domain of current research for their promising applications: as antimicrobial agents in wound dressing, as topical creams to prevent wound infections and as anticancer agents. Microemulsions, consisting of water droplets dispersed in oil and stabilized by surfactant monolayer served as nanoreactor and therefore has been an ideal template to control particle nucleation, growth, stability and aggregation. This concept has been successfully applied to prepare AgNPs with tunable size as well as controllable stability and aggregation by proper choice of different components and compositions to control dimension of water droplets of microemulsions.

24. Metal Oxide based hybrids for highly enhanced electrocatalytic product of Hydrogen, the future fuel

Soumyabrata Roy, Rajkumar Jana and Sebastian C. Peter
Solid State and Inorganic Chemistry Laboratory, New Chemistry Unit, Jawaharlal Nehru Centre of Advanced Scientific Research, India.

Polyoxometalates (POMs), a class of redox facile metal-oxy anion clusters, are strongly emerging as efficient, cheap, precious-metal-free electrocatalysts for hydrogen evolution reaction (HER). We have synthesized, three decavandate (V_{10}O_{28}^{6-}) based supramolecular inorganic-organic hybrids (1, 2 and 3) using different ligands (2,2’-bipyridine: 1, 4-amino pyridine: 2, and ethylene diamine: 3) and Cu as the secondary transition metal (in two of them, 1 and 2) for electrocatalytic HER applications. 3 exhibited excellent HER activity as cathode in acidic media with an onset overpotential of only 80 mV. The comparative activity order followed as 3>2>1. The trend suggests that there is a synergistic effect of both the transition metals (Cu and V) towards the catalysts’ HER activity.
References


25. KIT signaling regulates perinatal oocyte development in the mouse ovary

Joshua Burton and Melissa Pepling
Syracuse University, Syracuse

The pool of primordial follicles present at birth represents the total population of gametes available to a female throughout her reproductive life. Signaling mediated by the KIT receptor is important for many aspects of ovarian development, but its role in follicle formation is not well characterized. Using mouse ovary organ culture, we examine signaling pathways downstream of KIT to determine which have regulatory roles in follicle assembly. Our observations point to the molecular mechanisms that regulate oocyte development, and may serve to better elucidate the etiology of reproductive disorders like primary ovarian insufficiency. Research supported by NIH R15 075257.

26. Engineering a DNA molecular device as a “Plug-and-Play” biosensing platform

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DNA is a good design material for engineering molecular devices due to the well-understood Watson-Crick base pairing and predictable sequence-structure relationship. Also, DNA devices can interface easily with biological systems for autonomous bio-detection and imaging. As an example, we will present our “split proximity circuit” and share simple guidelines which can be used as a starting point for researchers interested in DNA designs. On the application front, we have demonstrated that our circuit can be used in a “plug-and-play” format to detect a wide range of biomolecules, including DNA, microRNA, protein and cell surface receptor clusters.

27. Utilisation of Syndecan-2 by dengue virus during infection of brain endothelial cells

Fakhriedzwan Idris, Siti Hanna Muharram, Zainun Zaini, Suwarni Diah

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Dengue virus (DENV) binds to diverse molecules in early infection and have been shown to use syndecan-2 for cell entry in lymphoid cells. Here, we explore syndecan-2 as a potential target receptor during infection of brain endothelial cells (bEnd.3). We infected syndecan-2-treated bEnd.3 monolayer with DENV1-4. Infected cell population was determined using flow cytometry 4 days post-infection with co-localisation study using immunofluorescence assay for confirmation. Our results showed a significant interaction and co-localisation for all serotypes. However, there was no complete inhibition. In conclusion, DENV targeted syndecan-2, but not as primary receptor, in the early infection of brain endothelial cells.


Ijugila Thilza

University of Bristol, UK

Bovine tuberculosis (bTB) is a zoonotic disease caused by mycobacteria bovis and possesses a great threat to the public. A face-to-face closed ended questionnaire was administered to 198 randomly selected abattoir workers for the study and data was collected and analyzed using descriptive and chi-square statistic with SPSS version 21.0. The mean age of respondents was 35.50±11.60. Awareness of bovine tuberculosis was found to have significant \( p \leq 0.05 \) associated with age, gender, marital status, level of education, job category, working experience, TB screening, history of cough, history of household treatment for TB and vaccination history of household. It was observed that abattoir workers indulge in risky behavior that exposes them to bTB and knowledge of bTB is acquired over long periods of working in the abattoir but the mode of contracting the disease is not totally known as many think only meat is a vehicle of bTB. This clearly shows that butchers and other abattoir workers need to be trained on bTB and existing policies governing the abattoir in the country should be enforced.

Key words: Bovine tuberculosis, abattoir, awareness

29. Influence of ascorbic acid on iron, zinc and calcium bioavailability in selected food samples

Poonam Singh, Surendra Prasad

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Ascorbic acid (AA), also known as Vitamin C, is water soluble and easily oxidized by air, heat and light. Fruits and green leafy vegetables are good source of Vitamin C. The study on addition of 5 mg and 10 mg AA in selected food samples showed significant increase in the bioavailability of iron, Zinc and Calcium. Chick peas, red kidney bean, green gram and wholemeal bread samples were digested \textit{(in vitro)} and analyzed for bioavailability of iron, Zinc and Calcium using Atomic absorption spectrometer. Except Chick peas iron bioavailability other samples showed increase in iron, zinc and calcium bioavailability percentage.

30. Inherent Safety Assessment Technique and Hazard Mitigation Framework for Early Stage of Process Design

Syaza Izyanni Ahmad
A safety program that prevents hazards from occurring is preferable compared to the typical approaches of eliminating hazards upon being detected. Manufacturing plants should be designed so that they are user-friendlier and exhibit good safety features to prevent accident. This can be done by preventing the presence of the hazards in the process during its design stages or also known as the inherent safety concept. This research proposes an inherent safety assessment technique through the application of logistic function followed by a hazard mitigation framework through the application of thematic analysis for inherent safety assessment during the early design stage.


Nadia Shardt and Janet A. W. Elliott
University of Alberta, Edmonton, Alberta, Canada

My research examines nanoscale phenomena from a fundamental thermodynamics perspective to develop predictive equations. It is relevant in fields ranging from drug delivery to atmospheric physics to separation technologies. One significant application of my research is to better quantify the effect of cloud condensation nuclei on weather patterns and climate. These nuclei upon which water condenses can have radii on the order of nanometers. Their properties determine the size and lifetime of clouds, which impact the amount of radiation transmitted to the Earth’s surface and the amount of precipitation. Nanoscale processes thus dictate global weather patterns.

32. Self-compacting in-situ cast Mud-Concrete load bearing walls

Rizna Arooz
University of Moratuwa

‘Soil’ is a natural and sustainable building material which possess endless advantages in construction. Conceptually, this material can be used to combine traditional elements in contemporary context. A greater understanding of the behaviour of the material will enable to redefine of its suitability to different types of novel construction which could cater to local demands. Thus, the attempt is to introduce the novel technique of self-compacting in-situ cast Mud-Concrete load bearing wall system to construction industry. This novel walling concept could answer the burning issues of housing crisis, energy demand, material scarcity, environmental deterioration, high construction cost and the urge of faster building technology especially took place in developing countries.

33. Optimal Control design framework of Hybrid Scooter Power-train suitable for Personal transportation

Himadri Das
Imperial College London, UK

India has witnessed a healthy market growth (around 16% YoY) of two wheeler scooter vehicles. This segment of vehicle is accepted by customers for personal transportation, due to ease of driving in
urban driving scenario. However, there is a scope of improving the system level efficiency by integrating electric traction system with the current power-train configuration.

The research focuses on the optimal control of the energy flow from the Internal combustion engine and electric traction system to reduce overall fuel flow consumption. The optimal control framework proposed in this work, is based on the dynamic programming methodology nested by the particle swarm optimization technique. This framework guarantee the minimum fuel consumption for the scooter power-train which is designed with multi-objective design criteria in mind.

34. Nanotechnology: A solution for high purity drinking water
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²University of South Africa, Nanotechnology and Water Sustainability Research Unit, College of Engineering, Science and Technology, Florida Science Campus, Roodepoort, South Africa

Our work is motivated by the poor water quality in South Africa where in rural areas water is abstracted and used without purification. Currently, nano-engineered membranes are synthesised for application in solar driven water purification systems as well as sea/brackish water desalination. In addition, portable household water purification systems are fabricated for application in rural areas of low income countries. Attention is also paid on graduate training programmes where unemployed youth as well as water process controllers are extensively trained on water treatment processes as well as water conservation. War on leaks projects are also conducted for water conservation purposes.

Keywords: nano-engineered membranes, desalination, water conservation, water purification

35. Combating climate change with nanotechnology
Jacob Martin¹, Radomir Slavchov¹, Edward Yapp², Jethro Akroyd¹, Sebastian Mosbach¹ and Markus Kraft¹,²
¹Department of Chemical Engineering and Biotechnology, University of Cambridge
²School of Chemical and Biomedical Engineering, Nanyang Technological University

The problem of climate change is not limited to the CO₂ produced, but extends to soot, the particulates that are contributing to the blackening of global ice and increasing its melting rate. We are yet to understand how soot forms in a flame and central to this quest is an understanding of the atomic arrangement of carbon in these molecules. We present evidence that soot has a nanostructure related to the cage-shaped fullerene C₆₀, and explore what impact this has on the formation and destruction of soot.

Keywords: Nanotechnology, combustion, soot, activated carbon

36. Modelling and optimization for one-way electric-car-sharing service
Xu Min
37. Scale-Selective Reduced Precision for More Efficient Forecasts of Weather and Climate

Tobias Thornes

University of Oxford, UK

Accurate weather forecasts are becoming increasingly important as the world struggles to adapt to climatic change. Forecast quality is limited by the resolution and complexity of the numerical models that forecast centres are able to run, and hence by the size of the computers they can afford. Conventionally, these models use double-precision (64 computer bits per number), but this may waste resources, especially when representing smaller-scale phenomena that are observed less accurately. We present results suggesting that up to 75% computational cost savings are achievable without affecting forecast accuracy by scale-selectively reducing precision, potentially freeing resources to produce better forecasts.

38. A birds-eye view of Southern Ocean change

Kalinka Rexer-Huber

University of Otago, New Zealand

The Southern Ocean is a notable challenge for sustainable management of marine resources: a circumpolar hotbed of fisheries management issues, and among the first systems to show climate change impacts. Changes in this very large ecosystem can be monitored via wide-ranging marine seabirds. I show how studies of white-chinned petrels, ranging around the Southern Hemisphere, provide insight into fisheries bycatch impacts via at-sea distribution, island population data, and genetic tools. Our data highlight important regions of accidental seabird bycatch in commercial fisheries, and provide baseline context to help assess the impact of other threats and changes in the Southern Ocean ecosystem.

39. Density-dependent colonization and natural disturbance limit the effectiveness of invasive lionfish culling efforts

Nicola S. Smith, Stephanie J. Green, John L. Akins, Skylar Miller, and Isabelle M. Côté

Simon Fraser University, Bahamas

Culling is used in the Caribbean to control invasive lionfish on coral reefs. Although frequent culling reduces lionfish abundance and halts native prey fish decline, the effectiveness of infrequent culling is
unclear. We found that infrequent culling reduced lionfish density by 60% - 79%, but did not stem prey decline. After a hurricane, lionfish densities became greater on all culled reefs, while native prey declined. The culling frequencies examined therefore offer a poor trade-off between the conservation gains achievable with frequent culling and the time and money saved by infrequent culling. Moreover, stochastic events like hurricanes can limit culling effectiveness.

40. How Grade 12 Students Misinterpret Tree Diagrams

Robin Seoh
Nanyang Technological University, Singapore

Biology learners have difficulties deriving accurate information from tree diagrams used in textbooks. In this study based on Grade 12 students, we primarily administered an open-ended question regarding the relationship between humans and chimpanzees, secondarily derived a checklist of organisms, and interviewed thirteen students, reporting nine alternative interpretations (mental pictures) of human phylogeny, a process aiming to make the mental models of learners more explicit. The findings were analysed in relation to the abstract nature of concepts of evolution, prior knowledge, as well as the alternative language-related schema encircling the various terms and conceptions adopted in the reading of tree diagrams.

41. Fish decline in the Lagos Lagoon, Nigeria: Impacts of saw-milling activities on *Clarias gariepinus* (African Mud Catfish) embryos

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The Lagos Lagoon receives wastes from various sources including saw-milling activities which are point sources of pollutants. The aim of this study was to investigate the impact of saw-milling activities on the Lagos lagoon on *Clarias gariepinus* embryos. The results showed that PAHs originated mainly from combustion sources with a dominance of high molecular weight PAHs in the surface water, sediment and pore water. Developmental abnormalities and decreased hatching success were observed in *C. gariepinus* embryos exposed to sediment organic extracts and pore water from the test site. Strict enforcement of waste management laws is recommended for the Lagos lagoon.

**Key words**: *Clarias gariepinus*, Lagos Lagoon, Nigeria, Polycyclic Aromatic Hydrocarbons (PAHs), Saw Milling Activities

42. Halogen bonding involving aromatic acceptors

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Halogen bonding (XB) has received renewed interest recently, with many theoretical studies themed on lone-pair-type XB donors. XB is also manifested in various fields such as crystal engineering, organocatalysis, functional materials, and drug design. A survey of structures within the protein data bank (PDB) revealed 33% of XB interactions involve close contacts between \( \pi \)-systems and a halogen (X) group.\(^1\) Our survey of crystal structures in the Cambridge Structural Database (CSD), shows 66% of the total XB close contacts involve \( \pi \)...X interactions, of which 96.5% involve aromatic rings. Delocalization of \( \pi \)-electrons on the plane of the ring make the attribution of favorable XB sites on the conjugated system a difficult task, in contrast with the straightforward case in lone-pair type XBs. We report here, the locations of favorable XB binding sites involving Cl\(_2\) as an XB donor, with different polycyclic aromatic hydrocarbons (PAHs) and heteroaromatic compounds as XB acceptors, deduced from PES scans using dispersion-corrected DFT, which in turn will provide useful insights into molecular assembly in functional material synthesis and applications.


43. Development of adaptive sampling technique for smart designing of computational experiments

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In this poster, we present our Smart Sampling Algorithm (SSA) for construction of global high dimensional surrogate models. SSA consists of a novel strategy to select sample points systematically in an adaptive and optimized manner that ascertains the placement in the most unexplored regions of the domain with complex/nonlinear behaviour. It iteratively solves the point placement optimization problem comprising of crowding distance metric and departure function. Finally, our numerical evaluation of SSA for a test function bed as well as process systems engineering case studies shows its excellent performance compared to the conventional techniques.