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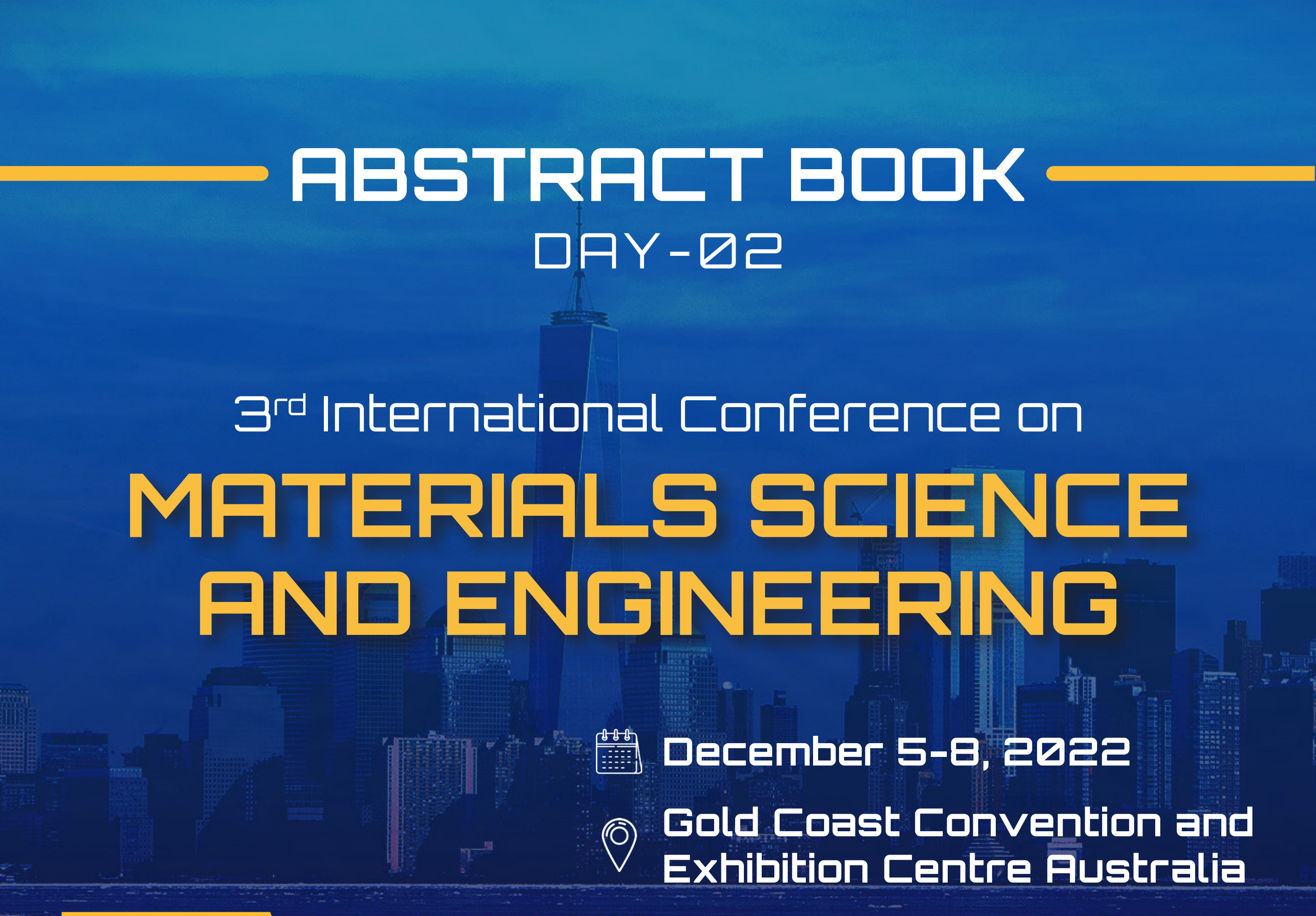

ABSTRACT BOOK

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Session: Nanotechnology and Nanoscience

Tailoring the Functionality of Topological Transistors by Targeted Materials Choices

Dimitrie Culcer[a,b]

[a]School of Physics, UNSW Sydney, Sydney 2052 NSW, Australia

[b]Australian Research Council Centre of Excellence in Future Low-Energy Electronics Technologies, UNSW Sydney, Sydney 2052 NSW, Australia

Topological transistors represent a new quantum paradigm in transistor design. They rely on edge states that exist in certain materials, in which up and down spins travel in different directions, and which can be turned on and off electrically using a topological phase transition [1, 2]. In this talk I will show that topological transistors offer unprecedented opportunities, and the choice of material plays an important role in determining their properties. The first of these is the sub-threshold swing, which is the fundamental critical parameter determining the operation of a transistor in low-power applications such as switches. It determines the fraction of dissipation due to the gate capacitance used for turning the device on and off, and in a conventional transistor it is limited by Boltzmann's tyranny to kTln(10)/q, or 60 mV per decade. I will show that the sub-threshold swing of a topological transistor in bismuthene can be sizably reduced in a non-interacting system by modulating the Rashba spin-orbit interaction via a top-gate electric field. We refer to this as the Topological Quantum Field Effect and to the transistor as a Topological Quantum Field Effect transistor (TQFET) [3]. The Rashba interaction can reduce the sub-threshold swing by more than 25% compared to Boltzmann's limit in currently available materials, but without any fundamental lower bound. I will discuss extensions of this idea to optimising topological switching [4] and combining topological transistors with negative capacitance materials [5]. Next, I will demonstrate the way the mobility can be enhanced in topological transistors made out of Na3Bi by applying a magnetic field [6, 7], which exhibits a non-trivial interplay with the strong spin-orbit interaction in this material [8]. I will show that a magnetic field also enables a strong non-linear response in a number of topological materials [9], including Na_3Bi and WTe_2.

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Ambipolar Control in Resistance Driven by an Electronic Attractive Force Using VO_2 Nano-bridge Transistors

Teruo Kanki[a*]

[a]*Osaka University: Mihogaoka 8-1, Ibaraki, Osaka, 567-0047*

Electric manipulation of spin, lattice and charge degrees of freedom in correlated electron materials based on transition metal oxides (TMO) offer original approaches toward non-conventional electronic and spin functions because TMO show dramatic changes in physical properties through external stimuli. A lattice strain effect, which is one of the popular approaches, evokes the transition from insulator to superconductor, change of magnetic and conductive aspects and the metal-insulator-transition (MIT) accompanied by orders of magnitude changes in resistance. Among them, vanadium dioxide (VO_2) is a prototypical correlated electron material which profoundly undergoes the MIT with strong electron-lattice coupling between monoclinic (M) insulating states at lower temperature and a tetragonal (R) metallic state at higher temperature across the MIT. Thus, strain effect dramatically induces a completely different electro-conduction aspect. This research demonstrates ambipolar change in conductivity by bending single-crystal VO_2 nano-bridges due to application of an electrostatic attractive force using bottom gates in a three dimensional structure, that is, line-symmetric resistance curves with convex or concave shapes appear, which are dependent on crystal-orientation of [001] or [110] in rutile type-VO_2, respectively. Approach on three-terminal-electrical control of lattice strain in single-crystal VO_2 will lead to realize exotic electronic applications such as power-free switch, tunable resonators and so on.

Controlled Synthesis of Zeolites via Mechanochemical Route and Confirmation of their Framework with Use of Synchrotron Radiations

Atsushi Muramatsu,[a*] ***Kiyoshi Kanie,***[a] ***Ryota Osuga,***[b] ***and Mizuho Yabushita***[c]

[a]*International Center for Synchrotron Radiation Innovation Smart, Tohoku University, Sendai 980-8577, Japan*

[b]*Institute of Multidisciplinary Research for Advanced Materials, Tohoku University, Sendai 980-8577, Japan*

[c]*Faculty of Engineering, Tohoku University, Sendai 980-8579, Japan*

Controlled synthesis of zeolite materials has been accomplished by the combination of mechanochemical and subsequent hydrothermal reactions in aqueous solution.1) The initially formed solid is amorphous with hetero-atom linked with Si atom via O atom, so that the substitution of hetero-atom in zeolite framework has carried out with use of this amorphous precursor, during the conversion into crystalline zeolite by dissolution of precursory solid and re-crystallization. We have already succeeded to prepare hetero-atom substituted zeolites such as Ce-MFI, Fe-MFI, Fe-Al-MFI, Ce-CHA, etc. In the present study, Fe-MFI is focused on. 2) Generally, zeolite materials are normally synthesized in homogenous aqueous solution by a simple hydrothermal synthesis method. In this case, the homogeneity in composition and structure is not guaranteed in particular for more than 2 kinds of hetero-atoms incorporated one, because the concentration of each component ions in solution is independently changed by the precipitation of solids with processing time. In order to maintain their same concentration in the solution, the solid-solution complicated system is accomplished, where solid acts as a resource of ions. Fe-MFI has been prepared with various Si/Fe ratios via mechanochemical route, and then Fe-MFI as well as precursory amorphous solid has been investigated to confirm Fe-O-Si bond by X-ray absorption fine structure (XAFS).

Initially, SiO_2 and ⍰-Fe_2O_3 were charged into a Si_3N_4 pot and pulverized together using a planetary ball mill apparatus until disappearance of diffraction peaks derived from ⍰-Fe_2O_3 completely. As a result, Fe atoms in the amorphous composite had tetrahedral coordination geometry and linked with Si atom via O atom. Therefore, Si–O–Fe linkages were formed in the amorphous composite. The hydrothermal synthesis was then performed for the synthesis gel composed of the amorphous composite, Carplex, tetrapropylammonium hydroxide (TPAOH), KCl, and H_2O. The XRD measurement revealed the formation of MFI-type framework by the hydrothermal synthesis in all cases. Both of the gradual increase of peak intensity at 200 nm in the UV-vis spectra as well as broadening of the peak at 1082 cm^{-1} in the FT-IR spectra upon a decrease in the Si/Fe ratio indicated that a larger number of Fe atoms were incorporated in the zeolite framework at a lower Si/Fe ratio. Fe-substituted MFI-type zeolites were successfully prepared by the mechanochemical method. 2)

XAFS spectra of precursory amorphous were measured with different grinding time in the preparation by mechanochemical treatment. Pre-edge peaks of the spectra show change in ratio of tetragonal Fe against octahedral Fe. Clearly, tetragonal Fe, bonding with O-Si, increased in place of octahedral one. During grinding, Fe atoms are incorporated into Si-O-Si bond by exchange of Si to Fe. When XANES spectra of Fe-MFI with different aging time of re-crystallization are compared between by mechanochemical route and by conventional hydrothermal reaction, the mechanochemical Fe-MFI results in the shorter time requiring for the introduction of hetero-atoms in zeolite framework than that by conventional synthesis method. As has been reported elsewhere, 2) the mechanochemical method enables isomorphously substituting metals to be distributed more homogeneously in the zeolite framework, which is beneficial for applications of zeolites in catalysis and other fields.

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2D Materials for Sustainable Energy Conversion and Storage

Ziqi Sun, Queensland University of Technology, Australia

Anomalous Effect of Fluorous Surfaces Confined within a Nanochannel: Highly Efficient Desalination

Yoshimitsu Itoh[a,b,]*

[a]*Department of Chemistry and Biotechnology, Graduate School of Engineering, The University of Tokyo, 7-3-1 Hongo, Bunkyo, Tokyo 113-8656, Japan.*

[b]*Japan Science and Technology Agency (JST), Precursory Research for Embryonic Science and Technology (PRESTO), 4-1-8 Honcho, Kawaguchi, Saitama 332-0012, Japan.*

Water scarcity is one of the most important issues for human beings to solve, as only 0.01 % of the water on earth can be immediately used for our daily lives. Currently, many reverse osmosis membranes, that can be used for the desalination of salty water, have been developed. Now, researchers are looking for much higher efficiency by mimicking the function of aquaporin. Aquaporin is a membrane protein that can transport water rapidly through its sub-nanometer channel but does not permeate other molecules such as ions including protons. This function is ideal for desalination and many aquaporin-mimetic synthetic nanochannels have been developed to date.[1] However, it is still a big challenge to surpass the function of aquaporin. Here we report a fluorous nanochannel that can permeate water three orders of magnitude faster and aquaporin and still reflect salts.[2] Our nanochannels are made of one-dimensionally assembled fluorous macrocycles with a pore diameter >0.9 nm. If we simulate the performance of our fluorous nanochannels when assembled as a membrane, they largely surpasses that of existing desalination membranes. Surprisingly, the performance was much higher than that of aquaporin- or carbon nanotube-based hypothetical membranes. We think that such a high performance was realized by the water-cluster breaking function of the fluorinated wall together with electrostatically negative fluorous nanochannel.

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Revealing the amorphous-to-crystalline transformation in zeolite synthesis using high-energy X-ray total scattering measurement

Toru Wakihara[1,2]

[1] *Institute of Engineering Innovation, The University of Tokyo*

[2] *Department of Chemical System Engineering, The University of Tokyo*

Zeolites are a class of important porous materials that are widely used as catalysts in industrial fields. Although tons of artificially synthesized zeolites are produced annually, deep understanding of the amorphous-to-crystalline transformation process at a sub-nanometer scale involved in the synthesis of zeolites, especially in the early stage where amorphous solids are the dominant component, are still insufficient, due to the lack of effective characterization techniques to identify the amorphous structures. Pair distribution function (PDF) analysis, by which different interatomic distances can be derived from scattering data, is an alternative approach to give insights into the structure of materials covering short-to-intermediate atomic arrangement, and therefore is particularly useful to analyse the architecture of disordered materials, like liquids and glasses. The PDF analysis based on the *ex situ* high-energy X-ray total scattering (HEXTS) technique using synchrotron X-ray, featuring improved real space resolution, has been tentatively applied to the researches on the structural evolution in the zeolite precursors. Very recently, *in situ* HEXTS-PDF analysis has also been developed, which is expected to be a promising approach to track the structural evolution of amorphous precursors towards crystalline zeolites under the practical hydrothermal conditions. In this talk, two cases, i.e., synthesis of zeolite X and SSZ-13 zeolite, regarding the recent progresses on the elucidation of the structural evolution of the amorphous zeolite precursors using the advanced *ex situ* and *in situ* HETXS-PDF analysis will be introduced, which helps deepen the understanding of the crystallization mechanism of zeolites, and give ideas to develop new zeolitic catalysts with novel compositions and topological structures.

Guided Formation of Nanoparticles and Polymer Brushes on Nanocellulose

***Nasim Amiralian,* [a]* *L. Geurds,* [a] *J. Lauko,* [a] *A. E. Rowan*[a]**

[a]*Australian Institute for Bioengineering and Nanotechnology (AIBN), The University of Queensland*

Conductive hydrogels combine the electrical properties of conductive materials such as metallic nanoparticles, conductive polymers, or carbon-based materials with hydrogels' biomimetic features such as high water content and tuneable physical and chemical properties have become promising candidates for developing printable inks for biomedical and electronics industries. Nanocellulose (NC) is the primary building block of plants that gained significant attention as an additive in inks. NC displays time-dependent shear-thinning behaviour, assisting the extrusion process and ink deposition, essential for developing intricate patterns and structures with micrometre precision. In addition, the versatile surface chemistry of NC enables the stabilisation and synthesis of conductive materials such as metallic nanoparticles, supporting the ink formulation.

We demonstrate an optimised approach for the esterification while controlling the degree of substitution of the initiator grafted on the surface, maintaining the rod-like morphology, cellulose I structure and minimal loss of the degree of crystallinity. These surface-modified nanocrystals enable the grafting of polymer brush systems with controllable lengths and densities. NC morphology was not compromised after grafting and metal nanorods synthesising. Understanding how reaction variables control and impact the characteristic properties of NC and the degree of substitution guides the tailoring of the surface modification and, as a result, tuning the NC-metal brush systems properties for advanced high-tech applications in different industries including flexible electronics and biomedical.

Large-size, High-quality 2D Transition Metal Dichalcogenides Lateral Heterostructures by Mixed Molten-salt-supported Chemical Vapour Deposition

Ary Anggara Wibowo[a¶*], Mike Tebyetekerwa[¶b], Thien Truong[a], Anh Dinh Bui[a], Felipe Kremer[c], Zhongshu Yang[a], Sandra Saji[d], Yuerui Lu[a], Zongyou Yin[d], Daniel Macdonald[a], and Hieu T. Nguyen[a*]

[a]School of Engineering, The Australian National University, Canberra, ACT 2601, Australia

[b]Dow Centre for Sustainable Engineering Innovation, School of Chemical Engineering, University of Queensland, St Lucia, Queensland 4072, Australia

[c]Centre for Advance Microscopy, The Australian National University, Canberra, ACT 2601, Australia

[d]Research School of Chemistry, The Australian National University, Canberra, ACT 2601, Australia

A scalable growth of atomically-thin two-dimensional (2D) transition metal dichalcogenides (TMDs) with defect-free large-area surfaces is crucial for developing high-efficiency optoelectronic devices. Herein, we systematically report a method to grow large-area and high-quality MoSe$_2$ monolayers, MoSe$_2$-WSe$_2$, and WSe$_2$-MoSe$_2$ lateral heterostructures using molten salt-based chemical vapour deposition (CVD). First, we investigate effects of isolated inorganic (NaCl and NaNO$_3$) and organic (PTAS), mixed inorganic (NaCl/NaNO$_3$) and hybrid organic-inorganic (PTAS/NaCl/NaNO3) salt catalysts on the CVD growth and optoelectronic quality of MoSe$_2$ monolayers and its lateral heterostructures with WSe2 in MoSe$_2$-WSe$_2$ and WSe$_2$-MoSe$_2$ assemblies. In brief, our results show that molten salt catalysts generally support a high-quality and large-area growth of MoSe2 monolayers with a low defect density. The mixed inorganic (NaCl/NaNO$_3$) salt supports the growth of MoSe$_2$-WSe$_2$ lateral heterostructures but not their counterpart of WSe$_2$-MoSe$_2$. Meanwhile, WSe$_2$-MoSe$_2$ lateral heterostructures are optimally grown with the support of the hybrid organic-inorganic (PTAS/NaCl/NaNO$_3$) salt. These results are ascribed to the difference in the associated kinetic and thermodynamical mechanisms for the growths of MoSe$_2$ and WSe$_2$ as starting materials. The obtained lateral heterostructures have an average size of ~160 microns (including both monolayer materials). Finally, combining various micro and nanoscale characterization techniques, including micro-photoluminescence (PL) and hyperspectral PL imaging, micro-Raman, femtosecond time-resolved PL (TRPL) spectroscopy, transmission electron microscopy (TEM), and scanning TEM (STEM) equipped with energy dispersive x-ray spectroscopy (EDX), we confirm that the optoelectronic quality of the realized heterostructures and monolayers is improved compared to their mechanically exfoliated counterparts. The obtained high-quality, large-area 2D TMD heterostructures could be useful for various optoelectronic applications.

Delivery of Therapeutic Agents using Biopolymers

Lisbeth Grøndahl

School of Chemistry & Molecular Biosciences, The University of Queensland, Brisbane, Australia

Australian Institute for Bioengineering and Nanotechnology, The University of Queensland, Brisbane, Australia

The use of delivery systems to deliver therapeutic agents is a strategy used to enhance drug stability, reduce side effects, and target specific sites. The applications are vast and cover cancer therapy,

tissue regeneration, and vaccines. Depending on the application, different administration routes are required which put restrictions on the type of delivery system that can be used. The work presented will illustrate design parameters for delivery of a range of active agents for different applications. Polysaccharide-based materials are the focus of the work presented. Finally, the work will highlight challenges and pitfalls in characterisation of the delivery systems; the effect of release media; and method of evaluating release of therapeutic agents.

Controlling Solid-state Dynamics of Pharmaceutical Glasses

Kohsaku Kawakami[a,b]

[a]*Research Center for Functional Materials, National Institute for Materials Science, 1-1 Namiki, Tsukuba, Ibaraki 305-0044, Japan*

[b]*Graduate School of Pure and Applied Sciences, University of Tsukuba, 1-1-1 Tennodai, Tsukuba, Ibaraki 305-8577, Japan*

Although solid-state pharmaceutical products are generally manufactured using crystalline drugs, glassy state is sometimes employed for enhancing dissolution rate of drugs. As dissolution of the drug is one of the key processes to determine amount of drugs absorbed when it is administered via the oral route, vitrification is an important technology for developing poorly soluble drugs. However, difficulty in controlling physicochemical properties of pharmaceutical glasses frequently inhibit their use. Especially, their crystallization during storage is not acceptable, for which detailed understanding on their dynamics is required.

Induction time for crystallization of pharmaceutical glasses under isothermal storage can be understood solely as a function of T_g/T, where T_g and T are the glass transition and storage temperature, respectively1). However, variations in induction times found in literature for identical compounds under the same storage conditions are significantly large2), which may be explained by many reasons including difference in processing/thermal history, difference in the impurity profile, and difference in the surface area of the glasses.

Celecoxib glass is generally believed to crystallize, if it is heated in differential scanning calorimetry (DSC). However, it is influenced by its thermal history. Our DSC study revealed that optimum nucleation temperature of the celecoxib glass to a metastable form was located at -50 °C[3]). Thus, if it does not experience the low temperature, possibility of nucleation remarkedly decreases. Similar observations were made for many compounds including ibuprofen and loratadine, suggesting that control of the thermal history is extremely important for assuring physical stability of glassy products.

Relaxation is also an important process for understanding physical stability of pharmaceutical glasses. We have evaluated pair-distribution function of ritonavir glass to find that rearrangement of hydrogen-bonds proceeded during isothermal annealing just below T_g 4). It influenced crystallization dynamics just above T_g significantly. When the glasses are prepared by cooling from the melt, the cooling rate was found to be an important factor to determine the glass properties. Molecules with many rotatable bonds were found to be sensitive to change in the cooling rate5), presumably because it provides large degree of freedom for rearrangement of the glass structure. Detailed understandings on relationship between glass dynamics and molecular/glass structure enables precise control of performance of the glassy products.

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Systematic Synthesis of a Series of Glycopolymers Having N-acetyl-D-glucosamine Moieties for Evaluations of Lectin-carbohydrate Interactions

Koji Matsuoka[*,a, b, c]

[a]Division of Material Science, Graduate School of Science and Engineering,

[b]Medical Innovation Research Unit (MiU), Advanced Institute of Innovative Technology (AIIT),

[c]Health Sciences and Technology Research Area, Strategic Research Center, Saitama University, Sakura, Saitama 338-8570, Japan

A series of water-soluble carbohydrate monomers having different methylene numbers of polymerizable aglycons were systematically prepared from N-acetyl-D-glucosamine (GlcNAc). A known oxazoline derivative derived from a GlcNAc peracetate was condensed with various alcohols having the corresponding w-alkenyl function. The acetyl protection on the glycosides was deprotected by means of trans esterification in MeOH with NaOMe as a catalyst to give the desired water-soluble glycomonomers, respectively. Typical radical polymerization in the presence of ammonium persulfate (APS)—tetramethylethylenediamine (TEMED) in water was applied for the monomers with acryl amide as a regulator for adjusting the average distance between carbohydrate residues, a series of glycopolymers having various densities of GlcNAc residues was obtained. Regulation of the polymers showed two pivotal points: one is the effect of lengths between carbohydrate residues and the polymer backbone and the other one is the influence of average densities of carbohydrates in the glycopolymer. Carbohydrate—protein interaction by means of the glycopolymer library for wheat germ agglutinin (WGA) as a model protein was investigated and the highest Ka value was obtained when the glycopolymer having the longest methylene length and the ratio of 1:10 (sugar unit : acrylamide unit) was used as a substrate.

Melt mixing of PCL/PEG/curcumin-loaded PLA microspheres for the suture applications

***Xiaoxuan Deng*[a]*, Maree Gould*[a]*, Rajesh Katare*[b] *and Azam Ali*[a]*

[a]*University of Otago, Centre of Bioengineering and Nanomedicine, Faculty of Dentistry, 362 Leith Street, Dunedin North, Dunedin 9016*

[b]*Uiversity of Otago, Department of Physiology, School of Biomedical Sciences, 270 Great King Street, Dunedin North, Dunedin 9054*

Wound healing is a complex process critical in restoring the skin's barrier function. This process can be interrupted by numerous factors resulting in chronic wounds that represent a major medical burden. A surgical suture is an ideal device for achieving local drug delivery while securing wound closure. [1]. Despite the variety of commercial sutures available, none have the capacity to maintain their mechanical strength while delivering efficient anti-bacterial, anti-inflammatory and antioxidant properties [1]. In this study, curcumin was selected as an alternative to replacing chemical drugs, particularly antibiotics. Unlike antibiotics, curcumin is a natural product extracted from the common spice turmeric [2]. The aim of this study is to produce a curcumin microsphere-embedded surgical suture as a controlled drug delivery system to facilitate wound healing. Firstly, curcumin-loaded microspheres were produced by the solid-in-oil-in-water emulsion method [3]. The particle sizes, the drug loading capacity and encapsulation efficiency of the microspheres, as well as four different fabrication variables, were investigated. Subsequently, the curcumin-loaded microspheres were melt-extruded with biomaterials polycaprolactone (PCL) and polyethylene glycol (PEG) to obtain surgical sutures. During the microsphere production, it was found that the higher concentration of the water phase, the smaller the particle size became (Avg. 40 µm). Moreover, utilizing 3% w/v and below concentrations of the water phase could avoid the formation of aggregates after lyophilizing. The highest drug loading capacity and encapsulation efficiency of microspheres could reach 12.80% and 15.23% respectively. Furthermore, the suture sample had an excellent tensile property and displayed a smooth surface, which ascribed to the miscibility of PCL/PEG with curcumin-PLA microspheres. We hypothesise that the presence of curcumin-loaded microspheres embedded within the sutures will be non-toxic/biocompatible and able to accelerate wound healing.

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Instability-directed Architectural Design of Oxides and Heterojunction Nanostructures for Energy and Environmental Applications

Sajjad S. Mofarah[a*], Xiaoran Zheng[a], Hamid Arandiyan[b], Pramod Koshy[a*], C. C. Sorrell[a]

[a]*School of Materials Science and Engineering, UNSW Sydney: Street Address/Box Number, Sydney, NSW, 2052*

[b]*RMIT University: 124 La Trobe St, Melbourne, VIC, 3000*

State-of-the-art metal oxides (MOs) and their heterojunction nanostructures (HNs) are attractive classes of materials used for diverse energy-related applications including catalysts, photocatalysts, sensors, and batteries. The functionalities of the MOs and HNs dominantly depend on their defect densities, which are determined principally by architecture of the nanostructures. Therefore, there has been an increasing focus on tailoring the architectures of nanomaterials so as to simultaneously maximize and optimize their defect densities. One novel technique is the use of metal-based coordination polymers (MCPs) including metal-organic frameworks (MOFs) as precursors for the preparation of complex nanostructures (carbon, metals, MOs) with enhanced energy storage and catalytic performance. This can be achieved by synthesis of MCP nanostructures and their subsequent conversion into MO/HN by heat treatment in different atmospheres. The majority of conventional MCPs suffer from chemical, structural, and thermal instabilities, particularly on extended exposure to media of moderate corrosion and temperature. Therefore, an extensive effort has been made towards fabrication of MCPs with improved stability. These approaches require the application of high temperature and pressure that make the process expensive, time-consuming, and laboratory customized. The conversion of MCP into MO/HN involves the removal of volatile organic ligands leaving behind the MO/HN while the architecture of the MCP remains constant. Therefore, the resultant architecture of the MO/HN is determined by the original architecture of the MCP. Further, the MOs and HNs developed by MCP conversion usually exhibit relatively low defect densities owing to the necessity of high-temperature and pressure during the conversion procedure.

The present work reports a new strategy to address the preceding shortcomings by establishing a modified anodic chronoamperometric electrodeposition (MACE) method to fabricate highly unstable MCPs, as a precursor, for synthesis of MO and HN nanostructures. Therefore, the typical chemical instability of CPs, which is considered as a disadvantage, has been leveraged to control design of one dimensional (1D) to three-dimensional (3D) nanostructured architectures. This is accomplished through rapid disassembly of the MCP precursors in polar solvents at low temperatures and controlled re-assembly upon solvent evaporation with controlled kinetics. This can be followed by rapid conversion of MCPs into defect-rich MOs and HNs with unprecedented architectures and new levels of functionalities that are hardly obtainable using pre-existing techniques. As a comprehensive example, Ce-based coordination polymers (Ce-CP) will be thoroughly discussed. The high applicability and scalability of such method has demonstrated through fabrication of several atomically thin 2D holey nanosheets, hollow spheres, hollow octahedrons, hexagonal nanotubes, and 2D/3D CeO2-x and their heterojunction nanostructures. The MO and HN derived materials have been extensively used for various energy storage (e.g., pseudocapacitance and metal-air batteries), energy transformation (e.g., OER and HER), and thermo-catalysis (e.g., CO oxidation, ozonation) applications.

This work appears to be the first to report a simple, cost-effective, template-free, and low-temperature approach for fabrication of multiscale MOs and HNs with precisely controlled architectures via the manipulation of the kinetics of nucleation/growth of the MCPs. Therefore, this has the potential to form the basis for a large-scale and versatile route for the synthesis of inorganic nanostructures with controlled architecture and number of available active sites.

Harnessing Kinetic Energy via Electromechanically Active Polymers

Peter Sherrell,[1*] Andris Sutka,[2] & Amanda Ellis[1]

[1] Department of Chemical Engineering, University of Melbourne, Parkville, Victoria, Australia, 3010

[2] Institute of Materials & Surface Engineering, Riga Technical University, Riga, Latvia, LV-1048

By 2050, it is estimated that there will be over 100 billion devices connected to the internet. Over 50% of these are anticipated to be wearable, implantable, or remote devices. In order to power these devices, larger (higher energy density) batteries will be needed – however, this will lead to large footprint, heavy devices. Harvesting ambient (from motion, heat, and/or light) energy via electromechanically active polymers will emerge as a critical tool to supplement battery power, thus mitigating increases in battery size.

We have recently reported record efficiency ferroelectric polymer energy harvesters enabled by polarisation locking of polyvinylidene difluoride-co-trifluoroethylene (PVDF-TrFE) around a nanomaterial template.[1] We use this PVDF-TrFE energy harvester, as well as novel 2D ferroelectric materials,[2] as models to study ambient energy harvesting. This talk will delve into the complexity of energy harvesting from ambient energy, discussing the interplay between ferroelectric and electrostatic mechanisms within mechanical-to-electrical energy conversion.[3,4] We demonstrate that by tuning surface topography and internal interfaces, the energy harvesting efficiency of these systems can be dramatically increased.[5-7]

We discuss the implications of these findings for the design of future high energy and power density polymeric mechanical-to-electrical energy harvesting systems.

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Highly Efficient Flexible Organic Photovoltaic Modules for Sustainable Energy Harvesting Under Low-light Condition

***Soyeon Kim*[a*]**

[a]*Korea Institute of Materials Sciecnece(KIMS): 797 Changwon-daero, Seongsan-gu, Changwon-si, Gyeongsangnam-do, Republic of Korea 51508*

This study aims to expand the practical applications of large-area flexible organic photovoltaics (OPV), such that they retain their high stability and efficiency even under various weather conditions and external stresses. By developing polyethyleneimine derivative-based cathode interfacial layer (CIL) and non-fullerene acceptor (NFA) material in OPVs, the efficiency and stability decrease rapidly due to an undesirable interaction when these two materials are concomitantly applied. In this study, we designed a novel low-cost metal-mediated cross-linked non-conjugated polymer interfacial layer (c-PEIE) and improved the device performance and stability of flexible OPVs from the cell-to-module scale. c-PEIE CIL based flexible OPV cell achieves one of the highest power conversion efficiencies (PCE) of 16.45% and remarkable photostability, retaining 77.58% of its initial PCE for 110 h under continuous light illumination, while the conventional PEIE based cells realize a PCE of 12.58% and poor device stability. Accordingly, a 50 cm^2, large-area, flexible OPV module was also fabricated with an excellent PCE of 13.12% which is ⍰ 80% as efficient as small-area flexible cells. Notably, c-PEIE based OPV devices maintain high output power on cloudy days, which is a particular point of interest to efficiently harvest sunlight energy constantly. The tunable energy barrier and significant low-leakage current of CIL play a critical role in reducing open-circuit voltage and fill factor losses under low-light environments. Such energy sources can provide power efficiently all day long in low-light or cloudy environments to the Internet of Things wireless networks integrated with battery-independent photovoltaics.

Inverse Design of Polymer Membrane Structure for CO_2 Separation Using Junction Tree Variational Autoencoder

***Takumi Matsumoto*[a] *, Masaya Miyagawa*[b] *and Hiromitsu Takaba*[b*]**

[a] *Graduate School of Engineering, Kogakuin University, 2665-1 Nakano ,Hachioji, Tokyo, 192-0015, Japan.*

[b] *Department of Chemical Engineering and Environmental Chemistry, Kogakuin University, 2665-1 Nakano, Hachioji, Tokyo, 192-0015, Japan.*

In natural gas plants, separation process of containing CO_2 is an important to reduce the operating costs. Thus, an optimal CO_2 separation process should be selected. Membrane separation using polymer membranes need low energy compared to absorption and distillation methods. Therefore, a enormous number of studies have been reported for polymer membranes for a wide range of various gas separation systems. Further development of membrane materials based on existing membranes that exhibit high permeability and selectivity is desired to reduce separation costs. However, the numerous possible structures that polymers can take limit experimental investigations. Therefore, it is important to use machine learning methods to efficiently search for materials from the vast compound space. In the recently proposed unsupervised machine learning method Junction Tree Variational Autoencoder (JT-VAE), features of molecular structures are compressed and mapped into the latent space by the Encoder and the molecular structures are reconstructed by the Decoder. Therefore, JT-VAE can construct a latent space from which the features of the molecular structure can be extracted. In this study, the JT-VAE machine learning method is used to construct the extracted features of the polymer structure. The optimum polymer structure for gas separation is then inverse-designed by structure search from around the coordinates of the polymer structure that shows superior membrane performance in the latent space.

In order to construct a latent space with learned features of various polymer structures, about 970 000 polymer structures were used as training data and a polymer structure generation network was constructed in JT-VAE. A random forest regression model was constructed to assess membrane performance for polymeric structures without measured membrane performance data in the latent space, with the Morgan fingerprint of the polymeric structure as the descriptor and measured CO_2 and CH_4 gas permeability as the objective variables. Polymer structures with superior membrane performance in the latent space were input and polymer structures were searched for in the neighborhoods of their latent coordinates.

The correlation between the experimentally measured gas permeability for CO_2 and CH_4 and the predictions of the random forest regression was verified. As both coefficients of determination for the test data are above 0.95, the model can be built without over-fitting. In addition, even in areas with a small number of data, the training data and the test data provide equally accurate predictions. Therefore, the model is able to predict gas permeability even for unknown data. 6FDA-duraene, which has been reported as a polymer with excellent performance, was input into the latent space and a structure search was conducted around its coordinates. As a result, a promising polymer membrane structure were proposed, which are located on the upper right side of the Robeson plot.

Sb-substituted $Cs_2AgBiBr_6$/g-C_3N_4 Composite for Photocatalytic C(sp^3)−H Bond Activation in Toluene

***Xuying Li*[a]*, *Haoxin Mai*[a], *Dehong Chen*[a], *Rachel A. Caruso*[a]**

[a]*Applied Chemistry and Environmental Science, School of Science, STEM College, RMIT University, 124 Latrobe Street, Melbourne Victoria 3000, Australia*

Visible-light driven photocatalytic selective aromatic C(sp^3)−H bond activation is a sustainable and green approach to obtain value-added oxygenates. Recently, all-inorganic halide perovskites have been employed as promising photocatalysts but they are restricted by charge recombination and limited visible light absorption. In this research, we developed a Sb-substituted $Cs_2AgBiBr_6$/g-C_3N_4 composite and tested its application for visible-light photocatalytic toluene oxidation. Adding the Sb dopant to the perovskite extended the visible light absorbance of $Cs_2AgBiBr_6$ to 650 nm. In addition, the heterointerface between the $Cs_2AgBiBr_6$ and g-C_3N_4 gave a staggered band structure between the two components that effectively improved the charge separation. The visible-light photocatalytic toluene oxidation rate toward benzaldehyde obtained for the composite was over 20 and 70 times higher than that of either $Cs_2AgBiBr_6$ or g-C_3N_4 alone, respectively, with a high selectivity of over 96%. Development of such all-inorganic lead-free halide perovskite-based heterostructures for visible light photocatalytic organic transformations is expected to have wide reaching application.

Tailoring the Structural Properties of the Barrier Oxide Layer of Nanoporous Anodic Alumina for Iontronic Sensing

Cheryl Law,[a,b*] Juan Wang,[a,b] Satyathiran Gunenthrian,[a,b] Huong Nguyen Que Tran,[a,b] Khoa Nhu Tran,[a,b] Siew Yee Lim,[a,b] Andrew D. Abell,[b,c] and Abel Santosa,[b]

[a]School of Chemical Engineering and Advanced Materials, The University of Adelaide, South Australia 5005, Adelaide, Australia.

[b]Institute for Photonics and Advanced Sensing, The University of Adelaide, South Australia 5005, Adelaide, Australia.

[c]Department of Chemistry, The University of Adelaide, South Australia 5005, Adelaide, Australia.

Nanoporous anodic alumina (NAA) membranes are engineered in three distinct acid electrolytes at their corresponding self-ordering anodizing potentials. They exhibit a characteristic ionic current rectification (ICR) signal between high and low ionic conduction states due to the presence of hemispherical barrier oxide layer (BOL) closing the bottom tips of the cylindrical NAA nanopores. The ICR properties of NAA membrane is demonstrated to be affected by the thickness and chemical composition of BOL, and the pH of ionic electrolyte solution. Their rectification efficiency, which is determined by the ionic current associated with the flow of ions across BOL, increases with the thickness of BOL at optimal pH conditions. The iontronic sensing capability of NAA membranes is established by measuring the dynamic ICR signal shifts in response to gold-thiol binding. The inner surface of nanopores in NAA membranes is chemically modified with thiol-terminated functional molecules for selective detection of gold metal ions (Au^{3+}). The ICR characteristics of NAA membranes change dynamically when exposed to an increasing concentration of gold ions, revealing two working ranges: low and high analyte concentration with low limit of detection achieved at pico and micromolar level, respectively. The sensitivity of NAA-based iontronic sensing system is shown to increase linearly with the thickness of BOL. This study builds up the foundation for the application of NAA membranes in iontronic systems, unleashing potential applicability across various disciplines such as sensing, energy conversion and nanofluidics.

Engineering of Slow Light Lasing from Solid-state One-dimensional Nanoporous Photonic Crystals

Abel Santos,[a,b*] Satyathiran Gunenthiran,[a,b] Juan Wang,[a,b] and Cheryl Suwen Law,[a,b]

[a]School of Chemical Engineering and Advanced Materials, The University of Adelaide, SA 5005, Australia

[b]Institute for Photonics and Advanced Sensing, The University of Adelaide, SA 5005, Australia

Nanoporous anodic alumina (NAA) is an attractive platform material for photonic technologies and applications.1 NAA features arrays of well-defined, self-organized, hexagonally distributed cylindrical nanopores embedded in a matrix of aluminum oxide (alumina, Al2O3). As such, this unique nanoporous platform provides a flexible effective medium that can be engineered to harness distinct forms of light–matter interactions such as light confinement and recirculation, slow light, and selective reflection and transmission. However, demonstrations of narrow bandwidth lasing emissions from this optical material remain limited. One-dimensional NAA photonic crystals

are flexible platforms to develop solid-state lasing systems since: i) the range of lattice constant (period length) can be engineered with precision across the broad spectrum, from UV to IR; ii) and distinct forms of NAA-based PC architectures can be realized (e.g., microcavities, DBRs, GIFs) to harness distinct types of light–matter interactions (e.g., light confinement and recirculation, slow light, hybrid plasmonic–photonic modes). Here, we demonstrate that narrow bandwidth NAA-based gradient-index filters (NAA–GIFs) can be optically engineered to achieve high-quality visible lasing. NAA–GIFs fabricated by a modified sinusoidal pulse anodization approach feature a well-resolved, intense, high-quality photonic stopband (PSB). The inner surface of NAA–GIFs is functionalized with rhodamine B (RhoB) fluorophore molecules through micellar solubilization of sodium dodecyl sulfate (SDS) surfactant. Systematic variation of the ratio of SDS and RhoB enables precise engineering of the light-emitting functional layer to maximize light-driven lasing associated with the slow photon effect at the red edge of NAA–GIFs' PSB. It is found that the optimal surfactant to fluorophore ratio, namely 20 mM SDS to 0.81 mM RhoB, results in a strong, polarized lasing at ~612 nm. This lasing was characterized by a remarkably high quality–gain product of ~536, a Purcell factor of 2.2, a lasing threshold of ~0.15 mJ per pulse, and a high-quality polarization ratio of ~0.7. Our results benefit the advancement of NAA-based lasing technology for a variety of photonic disciplines such as sensing, tweezing, light harvesting, and photodetection.

Carbon Nanomaterial Sensitized TiO_2 Composites for Efficient Visible Light Photocatalysis

S. Amanda Ekanayake[a*], Dehong Chen[a], Rachel A. Caruso[a]

[a]*Applied Chemistry and Environmental Science, School of Science, RMIT University, 124 La Trobe Street, Melbourne, Victoria 3000, Australia*

To enhance the optical absorption of TiO_2 heterostructures while extending the lifetime of photogenerated charges, here we report the development of carbon nanomaterial based TiO_2 ternary composites by combining two different carbon nanomaterials with TiO_2. These ternary composites were prepared using a two-step approach via a combination of sol-gel technique and hydrothermal treatment using titanium isopropoxide as the precursor and varied carbon: TiO_2 ratio. Structural, surface, morphological and optical properties of the composite nanomaterials were analyzed using XRD, XPS, SEM, UV-Vis and PL. Photocatalytic activity of the optimized ternary composite was determined by degrading aqueous solutions of acid orange 7 (AO7) dye and tetracycline under visible light irradiation. Results revealed that the heterojunction formed between the first carbon nanomaterial and TiO_2 in the binary composite causes a reduction in charge carrier recombination rate in comparison with bare TiO_2. Addition of zero-dimensional carbon to these binary composites significantly enhanced visible light absorption of the resulting ternary composite. The ternary composite showed a ten-fold increase in photocatalytic degradation of AO7 and two-fold increase in tetracycline degradation compared to TiO_2. Intermediate products of AO7 and tetracycline degradation analyzed through LCMS revealed that no harmful byproducts were formed upon photodegradation. By determining the active radicals responsible in photodegradation via scavenger tests, we put forward a possible mechanism for enhanced photocatalysis demonstrated by the ternary composite. The improved visible light photoactivity was attributed to the synergistic effect of the photosensitising property and electron storing ability of carbon nanomaterials.

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