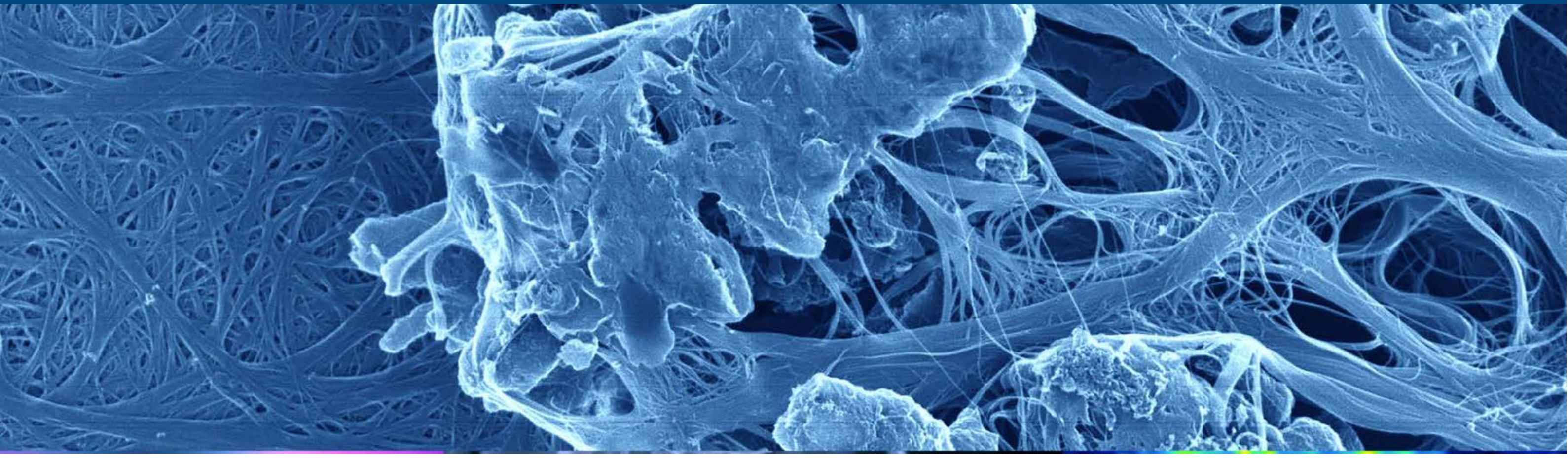
QUT ife Institute for Future Environments

NanoS-E3 2015

International Workshop & School

27 September - 2 October | Kingscliff, Australia

Nanostructures for Sensors, Electronics & the Environment



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Lectures’ Abstracts

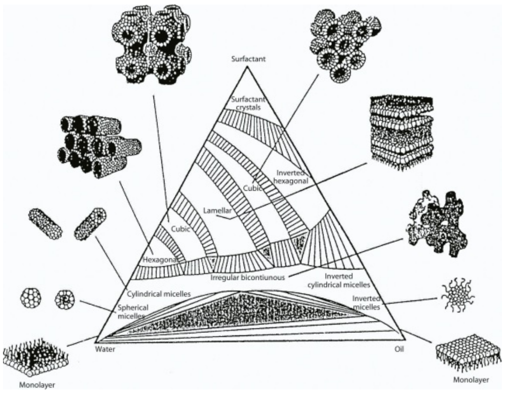
Interfaces, Surfactants and Self-assembly

Ian Gentle

The University of Queensland

In materials science, the presence of an interface between two phases or materials often has a strong influence over the properties of the material and how it interacts with its environment. This is particularly true in the field of nanoscience, where the basic functional and structural unit becomes smaller, the influence of the interface becomes even more significant. Because the interface is inherently a region of high energy, its presence can drive interesting and useful self-assembly behaviour, which is the basis of a number of mesoporous materials. The phase diagram below of a water/oil/surfactant system shows some of the fascinating shapes that are possible with simple surfactants and which are used in designing nanomaterials.

In this lecture I will discuss the properties of interfaces and how their properties can be modified and in particular investigate the use of the properties of interfaces in guiding self-assembly processes. A number of examples in materials science and catalysis will be given.



Reference: Interfacial Science: An Introduction, G.T. Barnes & I.R. Gentle, Oxford University Press, 2nd Edition, 2011.

Professor Ian Gentle

The University of Queensland Australia

Ian Gentle is Deputy Executive Dean, Faculty of Science and Professor of Chemistry in the School of Chemistry and Molecular Biosciences at the University of Queensland. Since arriving at UQ in 1993 he has led an active group working in applications of the physical chemistry of interfaces and his current research is in two main areas: organic optoelectronics applied to organic light emitting diodes, solar cells and sensors; and materials for energy storage, in particular lithium sulfur batteries.

Mono and Bidimensional Materials for Chemical Sensing

Guido Faglia

Sensor Lab, Department of Information Engineering,

University of Brescia & CNR-INO – Brescia - Italy

In solid state chemical sensing detection takes place at the gas/surface interface. Therefore novel materials mono (oxide nanowires) and bidimensional (graphene) are all surfaces materials suitable to develop innovative chemical sensors.

The lecture will critically assess performance, limits and outlooks of new dimensionally reduced materials for chemical sensing. Principles and mechamisms of detection are relatively known for oxide nanowires but yet unexplored for graphene and bidimensional materials.

Associate Professor Guido Faglia

Sensor Lab, Department of Information Engineering,

University of Brescia & CNR-INO – Brescia - Italy

Guido Faglia was born in 1965 and got in 1991 M.S. degree cum laude from the Polytechnic of Milan in electronics. In 1993 he was appointed Assistant Professor at the Gas Sensor Lab by the University of Brescia. In 1996 got the PhD on semiconductor gas sensors. Since 2000 he is Associate Professor in Experimental Physics at University of Brescia. In 2013 he got Italian Full Professorship habilitation as excellent in Condensed Matter Physics 02/B1 (see Annex I) . He is involved in the study of preparation of metal oxide semiconductors MOX as thin films and quasi monodimensional nanostructures for gas sensing, energy (solar cells, thermoelectrics), opto-electronic applications (LEDs) and nanomedicine. He has been involved in European Commission Projects since 1992 (Project ESPRIT No. 6374) in basic and applied physics research on semiconductors and their application in an interdisciplinary field as biochemical sensing. He has a relevant working experience with many international institutions like EC, NATO, European Space Agency ESA, INTAS. He is coordinating (2012-2015) the project WIROX in the frame of FP7-PEOPLE-2011-IRSES.

During his career Guido Faglia has published 171 articles on International Journals with referee (http://www.researcherid.com/rid/E-6991-2010). His Hirsch factor is 40 (Jul 2015); He is referee of many international journals among which Advanced Materials, Angewandte Chemie, Advanced Functional Materials and Sensors and Actuators B.

Electrochemistry

Anthony O'Mullane

Chair Electrochemistry Division Royal Australian Chemical Institute

School of Chemistry, Physics and Mechanical Engineering

Queensland University of Technology

The fabrication of nanostructured materials has recently received much attention due to their interesting optical, electronic, chemical and electrochemical properties. A popular method for creating such materials is using electrochemical approaches via either utilising an applied potential or manipulating the redox chemistry of the media employed. Advantages include the ease of fabrication, low cost, sample homogeneity and precise control over the size and shape of the required nanomaterial. The applicability of nanostructured materials created through electrochemical methods is quite extensive and includes electrocatalysts for fuel cells, heterogeneous catalysts, electrochromism, substrates for surface enhanced Raman spectroscopy (SERS), superhydrophobic surfaces and as sensing layers for electroanalytical applications to name but a few.

In this talk an overview is given on how electrochemical methods can be used to both fabricate and characterise a variety of metal and metal oxide nanostructures and how they can be utilised in the aforementioned applications. The versatility of electrochemical approaches is also demonstrated via the investigation of a newly introduced concept of liquid metal marbles that can be actuated under an applied electric field, utilised for heavy metal ion detection, photocatalysis, heterogeneous catalysis and as a pump without any mechanical parts.

Associate Professor Anthony O’Mullane

Chair Electrochemistry Division Royal Australian Chemical Institute

School of Chemistry, Physics and Mechanical Engineering

Queensland University of Technology

Anthony O’Mullane is an Australian Research Council Future Fellow and Associate Professor at Queensland University of Technology (Australia). He received his PhD degree (2001) from University College Cork (Ireland) and completed postdoctoral fellowships at Technische Universitat Darmstadt (Germany), the University of Warwick (UK), and Monash University (Australia). He previously held a position (2008) at RMIT University (Australia) until moving to QUT in 2013. He is currently Chair of the Electrochemistry Division of the Royal Australian Chemical Institute (RACI) and a Fellow of the RACI and Royal Society of Chemistry. His research interests are the electrochemical synthesis and characterisation of nanostructured materials; electrocatalysis; catalysis; semi-conducting charge transfer complexes; Li batteries; and the application of electrochemical methods to various aspects of physical, chemical and biological science. He has published 1 book chapter, co-authored 109 journal articles and 14 conference proceedings.

Fundamentals of Plasma Etching

Dr. David Lishan

Plasma-Therm,

Saint Petersburg - Florida 33716 – United States of America

David.Lishan@Plasma-Therm.com

These three lectures will focus on the fundamentals of plasma etching. Presentation material will review state-of-the-art etching technologies for applications in photonics, electronics, semiconductors, MEMS, materials research and nanofabrication. The first lecture will include an introduction to plasma processing, starting with a description of plasma, its generation, and the basics of plasma reactors. The differences between high- and low-density plasma systems will be reviewed in the context of why they were developed and how they are used. The majority of this first presentation will be an overview of etching mechanisms (physical, chemical, ion enhanced, and ion enhanced with passivation) with relevant examples. Utilizing the concepts discussed in the first presentation, the second and third talks will discuss current etching approaches for creating structures, with applications involving compound semiconductor and deep silicon etching.

Dr. David Lishan

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After receiving his undergraduate degree in Chemistry from UC Santa Cruz and Ph.D. from UC Santa Barbara in Solid State Electrical Engineering he has worked and published on a wide range of material, semiconductor, and chemistry R&D projects in the areas of lithography, photochemistry, x-ray mask fabrication, PVD, and plasma processing. During his nearly 17 years at Plasma-Therm, he has had business unit management and worldwide marketing responsibilities as well as managing the development of recently released plasma dicing product. Currently he is in the roles of Principal Scientist and Director in Technical Marketing, and recently organized and presented plasma processing workshops at leading institutions throughout the world. His primary focus is on the application of plasma processing for R&D, MEMS, photonics, data storage, power, and compound semiconductor applications. He holds two patents in the area of semiconductor processing and has over 60 publications and conference presentations.

With Plasma-Therm, he has organized and presented plasma processing workshops at leading institutions throughout the world, including Harvard University, UC Berkeley, University of Notre Dame, UC Los Angeles (UCLA), University of South Florida, Stanford University, Lund University (Sweden), IMRE (Singapore), UC Santa Barbara (UCSB), ISCAS (Beijing, China), SINANO (Suzhou, China), Shanghai Jiao Tong University, UT Austin, Cornell University, Pennyslvania State University, KANC (S. Korea), State Univeristy of Arizona, University of S. California, Xidian Univeristy, University of Alberta, and in Israel.

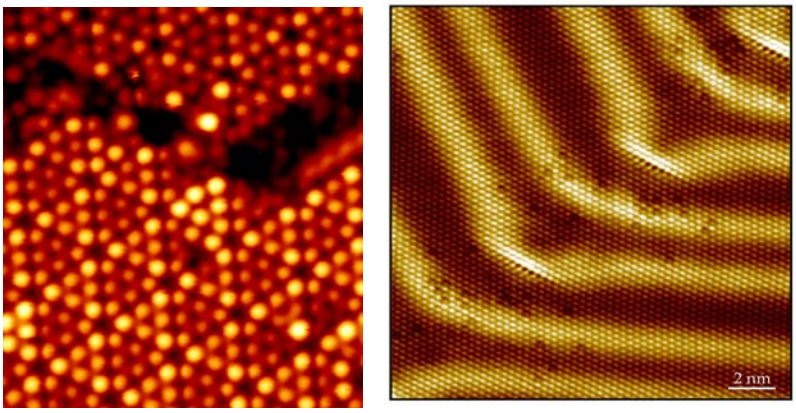
Introduction to Surface Science

Josh Lipton Duffin

Institute for Future Environments Queensland University of Technology, 2 George Street, Brisbane 4001, QLD, Australia

Surfaces and interfaces are everywhere and many surface-related phenomena are common in daily life (texture, friction, surface-tension, corrosion, heterogeneous catalysis). Understanding the microscopic properties of surfaces, asking questions like: what is the atomic structure of the surface compared to that of the bulk, is of utmost importance for modern technology. Surfaces are especially very important when dealing with ultra-small semiconductor structures is the field of nanotechnology. The electronic properties of nano structures are ultimately governed by quantum mechanics and the surface sets up the boundary conditions.

This lecture aims at providing a brief introduction to the physics of solid surfaces and to their experimental study. We will review the techniques and the instruments required to study the physics and chemistry of surfaces, and discuss the basic mathematical tools to describe surface phenomena.



SI 7x7 reconstruction (left) and Au(111) 3-domain herringbone reconstruction (right)

Dr Josh Lipton-Duffin

Institute for Future Environments

Queensland University of Technology

2 George Street, Brisbane 4001, QLD, Australia

Dr Lipton Duffin obtained his PhD in Physics at Queen's University Kingston, Ontario in 2006. He has strong skills in experimental techniques of surface science and associated instrumentation, with primary competencies in photoelectron spectroscopies (x-ray photoelectron and angle-resolved inverse photoelectron) and scanning tunneling microscopy (STM). He is proficient at epitaxial overlayer growth on metals and semiconductors, and has an extensive experience in LEED/Auger, X-PEEM and XRD both in laboratory and synchrotron environments. He published more than 45 papers in high impact factor International reviews (Small, ACS Nano, review of scientific instruments), with 457 citations and an h-index of 11.

At QUT since 2015 he is responsible of the surface science labs at the Central Analytical research Facility, conducting research in 2D materials and molecular self-assembly on surfaces.

Scanning Probe Microscopy and Molecular Self-Assembly

Jennifer MacLeod

CPME school and Institute for Future Environments Queensland University of Technology, 2 George Street, Brisbane 4001, QLD, Australia

The scanning tunneling microscope (STM) and the atomic force microscope (AFM), both capable of visualizing and manipulating individual atoms, are the cornerstones of nanoscience and nanotechnology today. The inventors of STM, Gerd Binnig and Heinrich Rohrer, were awarded with the Nobel Prize of physics in 1986. Both microscopes are based on mechanically scanning an atomically sharp tip over a sample surface, with quantum-mechanical tunneling or atomic forces between the tip and the atoms on the sample as the measurable quantities.

This lecture presents the principles of scanning probe microscopy, along with the experimental details. The mechanisms of atomic-scale imaging of both STM and AFM are discussed. The instrumentation and experimental techniques of STM and AFM, including piezoelectric scanners, vibration isolation, electronics and control, mechanical design, tip treatment and characterization, scanning tunneling spectroscopy, and atomic force detection techniques are explained in details. A number of examples related to molecular self-assembly and surface phenomena imaged by STM and AFM are presented.

Jennifer MacLeod

CPME school and Institute for Future Environments
Queensland University of Technology, 2 George Street, Brisbane 4001, QLD, Australia

Jennifer MacLeod holds a PhD in Physics from Queen's University in Kingston, Canada. Since receiving her PhD in 2006, she has worked as a Postdoctoral Fellow and Research Associate at the Centre Énergie, Matériaux et Télécommunications of the Institut national de la recherche scientifique (INRS-EMT, Varennes, Canada) and as a Natural Science and Research Council of Canada (NSERC) Postdoctoral Fellow at the Universita degli Studi di Trieste (Trieste, Italy). Dr. MacLeod specializes in condensed matter physics at the nanoscale, with particular interests in surface science and surface chemistry. Her primary research focus is on elucidating and controlling surface-confined molecular assemblies and reactions using a combination of high-resolution microscopy, spectroscopy and quantum chemistry calculations. She is also interested in instrument development, with the aim of developing new tools for nanoscale characterization and synthesis of materials. In February 2015, Dr. MacLeod joined the QUT School of Chemistry, Physics and Mechanical Engineering as a Senior Research Fellow in Surface Science.

Re-engineering the band-gap: searching for new phases of new phases of matter in silicon and diamond

D.N. Jamieson

School of Physics, ARC Centre for Quantum Computation and Communication Technology University of Melbourne – Parkville 3010 - Australia

It is now possible to fabricate devices which exploit the internal quantum degrees of freedom of single atoms in the solid state. These devices bridge the foundations of modern information technology based on silicon into the future of ultra-scaled devices where quantum mechanics offers new functionalities for information sensing, storage, processing and transmission.

Although silicon offers many advantages, a reappraisal of advanced theory for the band-gap of diamond suggests exotic magnetic phases of carbon may exist if suitable fabrication technqiues can be developed. In fact some controversial evidence has appeared in the literature for these exotic phases including superconductivity. These exotic phases may provide new physical processes for spin exchange coupling as well as a new superconducting pairing mechanisms that could be particularly robust.

Here we focus on the development of a technique that employs ion implantation that is compatible with the process flow for the fabrication of single atom semiconductor devices with the standard tools of the industry. The implantation of swift ions into semiconductor materials has a long history and the semiconductor industry presently employs many implantation steps in the fabrication of a typical large scale integrated circuit. It is therefore attractive to employ this standard technique for our purposes

This presentation reviews the theory, practice and results of ion implanted devices fabricated in silicon and diamond. A significant near-term challenge in silicon is to fabricate determistically implanted arrays of single atoms registed to control gates. In diamond the challenge is to use ion implantation to induce the magnetic phases and also to fabricate negatively charged nitrogen-vacancy centres (hereafter N-V) to act as the magnetic probes. In the near future, greater understanding of magnetic phenomena in carbon could lead to the ability to write magnetic circuits directly into a diamond host lattice of N-V qubits in a monolithic quantum device. Further improvement can be expected in the near future with increased understanding of the thermodynamics of these systems.

Acknowledgements: Supported by the ARC Centre of Excellence for Quantum Computation and Communication Technology and the ARC Discovery Project scheme.

During the presentation from David Jamieson at the NANOS-E3 School on Tuesday from 16:20 to 17:55 he will be conducting some online polls at various times. To participate in the polls you will need to connect to the webpage for your responses (address provided at the start of the presentation). Please bring your smartphone, tablet or laptop!

Professor David Norman Jamieson

School of Physics, ARC Centre for Quantum Computation and Communication Technology
University of Melbourne – Parkville 3010 - Australia

David is a Professor of Physics at the University of Melbourne. He completed his PhD in physics at the University of Melbourne in 1985 and then spent 4 years working at Caltech (USA) and the University of Oxford (UK) as a postdoctoral research fellow. He served as the Head of the School of Physics from 2008 to 2013.

His research expertise in the field of ion beam physics applied to test some of the key functions of a revolutionary quantum computer constructed in silicon in the Australian Research Centre of Excellence for Quantum Computation and Communication Technology where he is a chief investigator and program manager.

He served as President of the Australian Institute of Physics from 2005 to 2006 and is a Fellow of the AIP and the Institute of Physics UK. From 2010 to 2012 he convened a national working group to develop the Decadal Plan for Physics in Australia which was submitted to the Academy of Science in December 2012. In 2013 he received an outstanding service to physics award from the AIP.

Occasionally he gives public lectures on fundamental issues in physics.

School

Student Abstracts for Poster Presentation

Single-walled Carbon Nanotubes-Black Silicon Solar Cells Fabrication

Hawazn Abuhasha and Joseph Shapter1

Flinders Centre for Nano Scale Science and Technology, School of Chemical and Physical Sciences. Flinders University, Adelaide, Australia

Black silicon (B-Si) derives its name from its poor reflective and good absorbance properties, given by its rough surface morphology [1]. This morphology is created by dry-etching or wet-etching conventional silicon wafers to facilitate formation of a surface layer of nanostructure in form of whiskers, trenches, or pyramids. Recently, black silicon based solar cells achieved 22.1% efficiency[2].

Carbon Nanotubes (CNT) are semiconducting with a very small band gap, high aspect ratio, high conducting properties and unique electronic and mechanical properties. CNTs based solar cells achieved up to 14% efficiency [3].

The aim of this work is to combine both materials CNTs within B-Si to fabricate a new design of photovoltaic devices. Since CNT films can be used as transparent electrodes in light harvesting devices, CNT-silicon solar cells can be made by depositing CNTs on the surface of moderately doped n-type silicon substrates. Forming nanostructures in the surface of silicon substrate will make the solar cell black reducing the light reflection. Using black silicon (n-type) as the solar substrate and attaching a layer of CNTs as the front electrode will improve the electrical properties of the cell leading to increase in overall efficiency of the cell performance. This design will help in obtain higher efficiency and helps to reduce the production cost.

Deraoui, A, Balhamri, A, Rattal, M, Bahou, Y, Tabyaoui, A, Harmouchi, M et al.
2013, ‘Black silicon: microfabrication techniques and characterization for solar cells

applications,' International Journal of Energy Science (IJES), vol. 3, no. 6, pp. 403-407.

Hele Savin1*, Päivikki Repo1, Guillaume von Gastrow1, Pablo Ortega2, Eric Calle2, Moises Garín2 and Ramon Alcubilla2Black silicon solar cells with interdigitated back-contacts achieve 22.1% efficiency" Nature Nanotechnology, 18,May (2015).Print.

Tune, D. D., Flavel, B. S., Krupke, R. and Shapter, J. G. (2012) 'Carbon Nanotube- Silicon Solar Cells'. Advanced Energy Materials, 2(9), 1043-1055.

Polyamide membrane embedded with functionalized single wall carbon nanotubes SWCNTs for water treatment

Nasser Alotaibi, Martin Johnston and Joe Shapter

School of Chemical and Physical Sciences, Flinders University Bedford Park, South Australia- Australia

Thin film composites (TFC) of polyamide were prepared via interfacial polymerization process. TFC layer was adsorbed a polysulfone/polyester support layer. Thin film of polyamide membrane was subjected to improve the membrane properties giving that carbon nanotubes (CNTs) have been shown to have fast fluid transport[1, 2]. Fast transport occurs not only through the inner core of the carbon nanotubes, but the hydrophobic surface of CNTs increase molecular motion as well[3, 4]. Generally, embedding CNTs into polyamide membrane has been done by dispersion of CNTs into the aqueous phase as reported[5]. CNT dispersion in an organic phase was also been reported[6]. In this work, thin films of polyamide were prepared via interfacial polymerization of m-phenyldiamne (MPD) in aqueous phase and trimesic acid chloride (TMC) in the organic phase. SWCNTs were functionalized and dispersed in a mixture of n-hexane and toluene. The modified membrane structures were characterized by FTIR and TGA. The membrane surface changed after SWCNTs addition in polyamide as measured by SEM and contact angle results. The performance of the membrane was determined by measuring the flux of 2000ppm of NaCl solution through the membrane. Salt rejection also measured for permeated water.

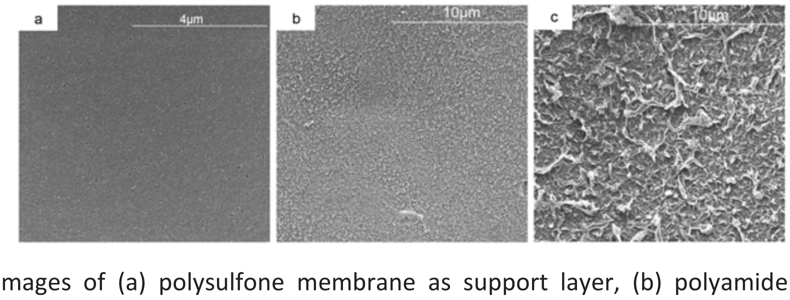


Figure 1, SEM images of (a) polysulfone membrane as support layer, (b) polyamide membrane with

SWCNTs-free in organic phase mixture (hexane/toluene), (c) polyamide/SWCNTs membrane with concentration of SWCNTs 0.076 wt. % in organic phase mixture (hexane/toluene).

Holt, J.K., et al., Fast mass transport through sub-2-nanometer carbon nanotubes. Science, 2006. 312(5776): p. 1034-1037.

Majumder, M., N. Chopra, and B.J. Hinds, Mass transport through carbon nanotube membranes in three different regimes: ionic diffusion and gas and liquid flow. ACS nano, 2011. 5(5): p. 3867-3877.

Zhao, H., et al., Improving the performance of polyamide reverse osmosis membrane by incorporation of modified multi-walled carbon nanotubes. Journal of Membrane Science, 2014. 450: p. 249-256.

Celik, E., et al., Carbon nanotube blended polyethersulfone membranes for fouling control in water treatment. Water research, 2011. 45(1): p. 274-282.

Yin, J. and B. Deng, Polymer-matrix nanocomposite membranes for water treatment. Journal of Membrane Science, 2015. 479: p. 256-275.

nan Shen, J., et al., Preparation and characterization of thin-film nanocomposite membranes embedded with poly (methyl methacrylate) hydrophobic modified multiwalled carbon nanotubes by interfacial polymerization. Journal of Membrane Science, 2013. 442: p. 18-26 .

Conjugation paclitaxel to functionalised gold nanoparticles for breast cancer treatment

Zahrah Alhalili1, Daniela Figueroa2, Barbara Sanderson2 and Joseph Shapter1

1 Flinders Centre for NanoScale Science and Technology, School of Chemical and Physical Sciences. 2 School of Medical Science and Technology, Flinders University, Adelaide, Australia

Paclitaxel is an anticancer drug (1). However, it has limitations such as non-specific targeting and insufficient dosages reaching the tumor which leads to severe side effects (2). Therefore, nanotechnology has emerged with novel materials exhibit unique properties (3). Among them, gold nanoparticles, AuNPs, have attracted significant attention due to their properties such as biocompatibility and non-cytotoxicity making them promising in medical applications (4).

The aim of this study was to develop a novel drug delivery system combines AuNPs with paclitaxel to improve the limitations exist in free paclitaxel.

AuNPs were synthesised by sodium citrate reduction method and the surface was functionalized using carboxylic- terminated thiol alkane. Then, paclitaxel was conjugated to AuNPs.

Fig.1. shows the FT-IR spectra of AuNPs capped paclitaxel. These results confirm the successful conjugation between paclitaxel and the functionalised AuNPs.
A cytotoxicity assay for AuNPs-paclitaxel conjugates was performed (Fig.2). T47D cells were treated with five different concentrations of the conjugates for 24 hours. T47D cell number was reduced significantly compared to the untreated control.

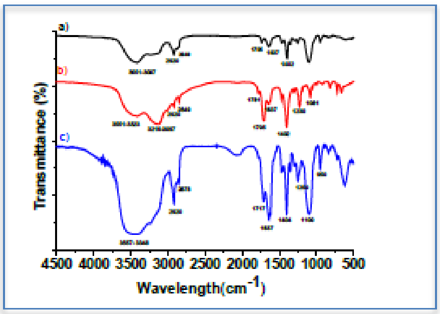


Fig.1. FTIR spectra of (a) 16-MHDA @ AuNPs, (b) NHS-16-MHDA @ AuNPs, (c) 16-MHDA@ Au NPs- paclitaxel conjugates.

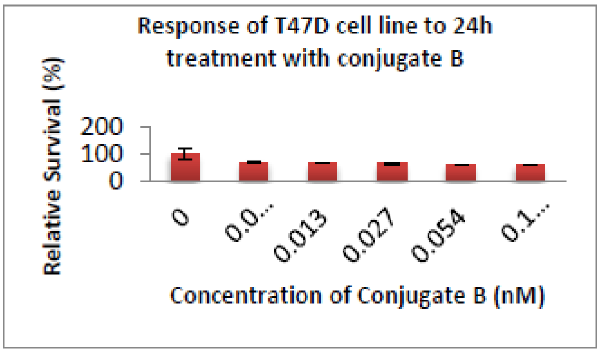


Fig.2. Response of T47D cells to 24h treatment with AuNPs- paclitaxel conjugates

1. Li, N., et al., Polysaccharide-gold nanocluster supramolecular conjugates as a versatile platform for the targeted delivery of anticancer drugs. Scientific Reports, 2014. 4[4164]: p. 1-7.
2. Wang, X., et al., Application of nanotechnology in cancer therapy and imaging. CA Cancer J Clin, 2008. 58[2]: p.97- 110.
3. Ochekpe , N., et al., Nanotechnology and drug delivery part 1: background and applications. Tropical Journal of Pharmaceutical Research, 2009. 8[3]: p. 265- 274.
4. Kumar, A. et al, Gold nanoparticles functionalized with therapeutic and targeted peptides for cancer treatment.Biomaterials, 2012. 33: p. 1180-1189.

Towards Semiconducting Graphene

Mojtaba Amjadi Pour1, Iolanda Di Bernardo1,2, Bharati Gupta1, Josh Lipton Duffin1, Carlo Mariani2, Maria Grazia Betti2, Nunzio Motta1
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Queensland University of Technology – Brisbane 4001 – Australia
2. Dept. of Physics Università di Roma La Sapienza – Rome – Italy.

Existing research recognizes the crucial potential of graphene use in electronics [1]. However, its remarkable range of applications has been challenged because of the fact that graphene is a semimetal with zero bandgap [2]. Therefore, over the past few years, a considerable amount of literature has grown up around the theme of producing a semiconducting graphene.

Quantum confinement in graphene nanostructures is one of the suggested pathways to achieve the opening the band gap by [3]. Substrate-induced [4] and strain-induced [5] techniques are also suggested in order to shift the band gap. Producing semiconducting graphene is also reported to be possible by changing the graphene crystalline structure. This can be performed by introducing defects, hydrogen passivation, boron and nitrogen doping and nanoscale holes creating nanomeshes.

Graphene has never been grown on nanometer-scale SiC mesas. Quantum mechanics suggests that electrical properties might change drastically by shrinking the size to the nanoscale. The aim of this project is to produce graphene on SiC mesas on Si with lateral sizes ranging from few tens of nm to 1 □m, and to st
properties of the graphene layer obtained. Two types of patterns will be generated using FIB on SiC structure; these patterns are depicted in Fig. 1.

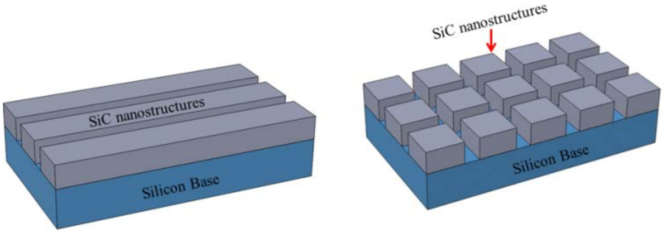

Figure 1, patterned created within 3C SiC structure.

1. Novoselov, K.S., et al., Electric Field Effect in Atomically Thin Carbon Films. Science, 2004. 306(5696): p. 666-669.
2. Novoselov, K., et al., Two-dimensional gas of massless Dirac fermions in graphene. Nature, 2005. 438(7065): p. 197-200.
3. Palacio, I., et al., Atomic Structure of Epitaxial Graphene Sidewall Nanoribbons: Flat Graphene, Miniribbons, and the Confinement Gap. Nano letters, 2014. 15(1): p. 182-189.
4. Zhou, S., et al., Substrate-induced bandgap opening in epitaxial graphene. Nature materials, 2007. 6(10): p. 770-775.
5. Blanc, N., et al., Strains induced by point defects in graphene on a metal. Physical review letters, 2013. 111(8): p. 085501.

Phases of Carbon: Boron-implanted Diamond

H. Bowers, B.C. Johnson, L.H. Willems van Beveren S. Prawer,

J.C. McCallum, and D.N. Jamieson

School of Physics, University of Melbourne – Parkville 3010 – Australia

We aim to investigate superconducting phases of heavily Boron implanted doped single crystal diamond, predicted to exist by a recent reappraisal of BCS theory in semiconductor materials. Bulk transitions are expected at 70 K [2] whilst localised regions may achieve transitions at 290 K [3]. Diamond, Boron Doped via growth processes were first seen to superconduct at 4 K in 2004 [4] with recent signatures discovered at 25 K [5].

The major challenge is to introduce boron into the diamond lattice above the metal-to-insulator transition density of 1×10^{21} atoms cm^{-3}[6]. We employ ion implantation at 600°C [7] followed by post-implantation annealing at 1450°C in vacuum – to electrically activate Boron and further repair the lattice. [8]

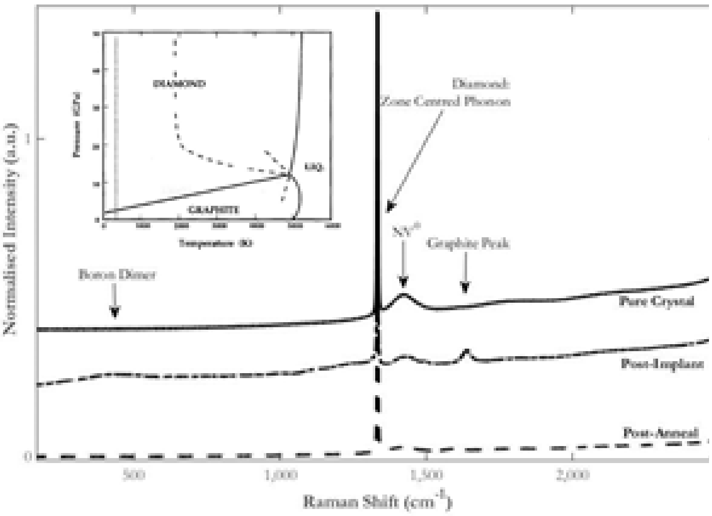

Figure 1: Raman Spectra of Implantation and Annealing upon 1e17(1MeV) with inset of Diamond Phase Diagram [1]

To date we have implanted device grade IIa diamond with fluences of 1×10^{17} (2MeV), 2×10^{16} (2MeV), 1×10^{17} (1MeV) and 8×10^{17}(1MeV) and have shown representative Raman spectra demonstrating lattice recovery, c.f. Fig. 1. Low-temperature magneto-transport measurements on van der Pauw devices reveal highly conducting sub-surface layers and signatures of superconductivity are being sought at mK temperatures.

The authors acknowledge access to ion-implantation and/or ion-beam analysis facilities at the ACT node of the Heavy-Ion-Accelerator Capability funded by the Australian Government under the NCRIS program, the Australian Research Council DP150102703 and Marvin L. Cohen for indispensable discussions.

[1] F. P. Bundy, W. A. Basset, M. S. Weathers, R. J. Hemley, H. K. Mao, and A. F. Goncharov, Carbon 34, 14 (1996).

[2] J. E. Moussa and M. L. Cohen, Physical Review B 77 (2008).

[3] M. L. Cohen, Journal of Materials Research 26, 2815 (2011).

[4] E. A. Ekimov, V. A. Sidorov, E. D. Bauer, N. N. Mel'nik, N. J. Curro, J. D. Thompson, and S. M. Stishov, Nature 428 (2004).

[5] H. Okazaki et al., Appl Phys Lett 106, 052601 (2015).

[6] E. Bustarret, P. Achatz, B. Sacepe, C. Chapelier, C. Marcenat, L. Ortega, and T. Klein, Philosophical transactions. Series A, Mathematical, physical, and engineering sciences 366, 13 (2008).

[7] N. Tsubouchi, M. Ogura, N. Mizuochi, and H. Watanabe, Diamond and Related Materials 18, 128 (2009).

[8] N. Tsubouchi and M. Ogura, Japanese Journal of Applied Physics 47, 7047 (2008).

Computational Design of Innovative Catalysts for Hydrogen evolution reaction

Guoping Gao

School of Chemistry, Physics and Mechanical Engineering Faculty,
Queensland University of Technology, Garden Point Campus, QLD 4001,
Brisbane, Australia

Traditional energy sources, fossil-fuels, use carbon and sulphur as energy carriers, which have resulted in unavoidable anthropogenic issues, including global warming, and acid rain1. To solve these environmental issues, a new environmentally-friendly energy carrier is highly desired2. Hydrogen, with the largest energy density and producing no pollution, is considered the ideal energy carrier3.

However, hydrogen element does not exist as hydrogen energy naturally. H2 produced by water splitting might be the ideal way to meet our environmental anticipation4. The graphitic carbon nitride (gh-C3N4) 5 and MoS26-7 are considered to be promising electrocatalysts for the hydrogen evolution reaction (HER). In this poster, I will show our recent results of HER on these two systems.

1. Armaroli, N.; Balzani, V., Energy for a sustainable world. Wiley-VCH, Weinheim 2011.
2. Walter, M. G.; Warren, E. L.; McKone, J. R.; Boettcher, S. W.; Mi, Q.; Santori, E. A.; Lewis, N. S., Solar water splitting cells. Chemical reviews 2010, 110, 6446-6473.
3. Dunn, S., Hydrogen futures: toward a sustainable energy system. International journal of hydrogen energy 2002, 27, 235-264.
4. Maeda, K.; Domen, K., Photocatalytic water splitting: recent progress and future challenges. The Journal of Physical Chemistry Letters 2010, 1, 2655-2661.
5. Wang, X.; Maeda, K.; Thomas, A.; Takanabe, K.; Xin, G.; Carlsson, J. M.; Domen, K.; Antonietti, M., A metal-free polymeric photocatalyst for hydrogen production from water

under visible light. Nature materials 2009, 8, 76-80.

6. Feldman, Y.; Wasserman, E.; Srolovitz, D. J.; Tenne, R., High-Rate, Gas-Phase Growth of MoS2 Nested Inorganic Fullerenes and Nanotubes. Science 1995, 267, 222-225.

7. Splendiani, A.; Sun, L.; Zhang, Y.; Li, T.; Kim, J.; Chim, C.-Y.; Galli, G.; Wang, F., Emerging photoluminescence in monolayer MoS2. Nano Lett. 2010, 10, 1271-1275.

Single-Walled Carbon Nanotube/Silicon Heterojunction Solar Cells

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Solar Cells with 7.7% photo conversion efficiency were fabricated using a known process. In addition a gold chloride treatment was shown to increase solar cell efficiency. It was also found that both metallic and semiconducting types of single-walled carbon nanotubes can lead to the production of a photocurrent, however they types may possess different inherent film morphologies.

In the last decade, novel photovoltaic cell designs have emerged making use of a carbon nanotube/silicon heterojunction to produce a photocurrent. This design improves on standard p-n silicon photovoltaic cells by replacing the, expensive to process, n-type silicon layer (or occasionally p-type layer) with a cheaper single-walled carbon nanotube (SWCNT) film[1]. The design used in this work is shown in Fig 1. Cells of this design were fabricated as a proof of concept before experimental alterations/doping procedures were performed, with efficiencies as high as 7.7% obtained.

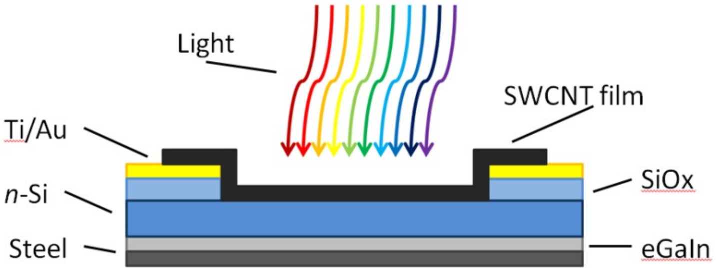

Fig 1: A standard Single-Walled Carbon Nanotube/Silicon Heterojunction Solar Cell, where the n-Silicon, with 100nm silicon oxide surface layer, substrate is attached to a steel place via a gallium-indium eutectic. The top surface of the silicon is patterned with 5 nm of titanium and 140 nm of gold with a central hole in the middle.

This hole is etched to allow the SWCNT film to contact the n-silicon.

The arrangement of carbon atoms within a carbon nanotube gives rise to two different electronic ‘types’ metallic, and semiconducting[2]. In this work the effect of nanotubes of different types on the photocurrent produced by the SWCNT/Si solar cell was tested, firstly by replacing the SWCNT film in the standard design (a mix of unsorted nanotube types) with a film consisting solely of metallic or semiconducting SWCNTs. A series of films of known semiconducting to metallic SWCNT ratios was also tested, to examine the effects of specific mixtures of semiconducting and metallic tubes. The results suggested that semiconducting tubes allowed the cell to produce a greater photocurrent than metallic tubes, however this was determined to be very likely due to imperfections in the films used, rather than the electronic properties of the tubes. The nanotube film morphology was examined using scanning electron microscopy and it was found that metallic SWCNTs formed less homogenous films than the semiconducting SWNCTs.

Additionally, the effect of a gold chloride solution as a nanotube dopant on cell performance was examined briefly in this work. It was found that the gold chloride can improve the efficiency of treated cells, however, the method and order of cell treatment greatly affects the end result and more work is required in this area.

1. Daniel D. Tune, Benjamin S. Flavel, Ralph Krupke and Joseph G. Shapter, Carbon Nanotube-Silicon Solar Cells. Advanced Energy Materials, 2012. 2(9): p. 1043-1055.
2. Tune, Daniel D, Blanch, Adam J, Krupke, Ralph, Flavel, Benjamin S, and Shapter, Joseph G, Nanotube film metallicity and its effect on the performance of carbon nanotube–silicon solar cells. physica status solidi (a), 2014. 211(7): p. 1479-1487.

Study of Si diffusion during the formation of epitaxial graphene layers on 3C SiC/Si (111)

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Compared to other synthesis methods, the growth of graphene in UHV on SiC gives origin to a contaminant free surface. Recently it has been shown that SiC/Si substrates are a good alternative to bulk SiC, allowing to reduce the cost and to better integrate the material with the Si based electronic devices. SiC/Si (111) substrate is the most suitable for the growth of graphene, due to its 3 fold symmetry, and will help to open the band gap of graphene [1].

The growth of graphene on in SiC in UHV has been discussed by many researchers [2], but there is still a lack of understanding regarding the kinetics of Si diffusion and its connection to the formation of graphene layers.

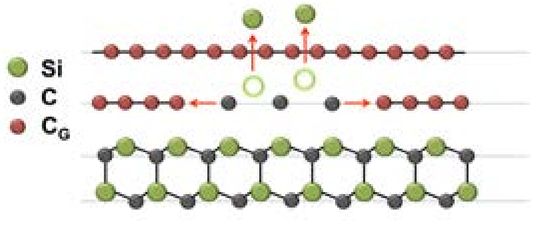

Figure 2 Schematic representation of epitaxial growth of graphene on SiC, according to the bottom-up mechanism.

In this study we analysed the number of graphene layers obtained on 3C SiC/Si (111) as a function of the annealing parameters by using X-ray Photoelectron Spectroscopy. We have grown graphene at temperatures ranging from 1175°C to 1350°C.

At each temperature the annealing sequence was monitored by acquiring high-resolution XPS spectra of the carbon peak at defined time intervals, obtaining a plot of the number of graphene layers as a function of annealing time [3].

We demonstrate how this growth is connected to the diffusion parameters of Si atoms in the matrix, and how it is possible to control the annealing process in order to obtain the desired number of epitaxial graphene layers.

[1] Novoselov, K.S., "Graphene: Mind the gap," Nature materials, 2007, 6, pp. 720-721.
[2] Ouerghi, A, et al., "Epitaxial graphene on cubic SiC (111)/ Si (111) substrate," Applied Physics Letters, 2010, 96, pp.
[3] Gupta, B., et al., “Evolution of epitaxial graphene layers on 3C SiC/Si (111) as a function of annealing temperature in UHV”. Carbon , 2014, 68, 563

Promoted Protein Adsorption and Cellular Attachment upon Nanostructured Au Surface

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Protein adsorption and cellular attachment are key research topics in the recent years. They are extensively investigated in many research fields, such as biosensors, drug delivery systems, implantable medical materials, and microfluidics [1, 2]. However, it is still not fully understood how nanostructures of material surface affect protein adsorption and ensuing cellular attachment.

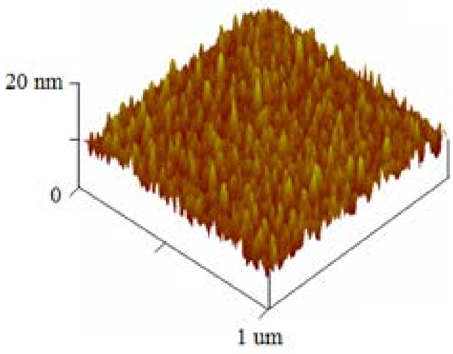

Figure 3 Au substrata

In this research, we investigated the adsorption of bone morphogenetic protein-2 (BMP-2) and ensued cellular adhesion of C2C12 cells on the Au substrate, whose nanostructures were up to 20 nm (showed on the right). The mass-uptake of BMP-2 was measured by a quartz crystal microbalance with dissipation (QCM-D) technique. The cytoskeleton of attached C2C12 cells was stained with FITC fluorescent dyes.

The results revealed that a 30% enhancement of adsorption amount was achieved on the nanostructured Au surface compared to the flat titanium (Ti) substrate. Moreover, the cellular adhesion of C2C12 cells was also promoted on the nanostructured Au surface compared to the reference Ti surface. It is believed that the nanostructures induced more specific adsorption sites [3], where BMP-2 molecules were highly favored to bind. With a robust loading of BMP-2, the Au surface therefore exhibited well-organized cellular attachments. Our findings enrich the mechanism of protein-surface interactions and highlight the potential use of small nanostructures (< 20 nm) in bone implants/scaffolds.

1. Kang, B., et al., Carbohydrate-Based Nanocarriers Exhibiting Specific Cell Targeting with Minimum Influence from the Protein Corona. Angewandte Chemie-International Edition, 2015. 54(25): p. 7436-7440.
2. Lacerda, S.H.D.P., et al., Interaction of Gold Nanoparticles with Common Human Blood Proteins. Acs Nano, 2010. 4(1): p. 365-379.
3. Schwab, E.H., et al., Nanoscale Control of Surface Immobilized BMP-2: Toward a Quantitative Assessment of BMP-Mediated Signaling Events. Nano Letters, 2015. 15(3): p. 1526-1534.

Single-Layer Sodium Phosphidostannate(II): A First-Principles Study

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Layered materials in their bulk forms have been well-known and utilized in device application for hundreds of years. Atoms in layered materials are strongly bonded in-plane but weakly interact out-of-plane through van der Waals forces. This weak interlayer interaction makes it possible to extract one or a few layers from their bulk forms, leading to burgeoning research on two-dimensional (2D) materials.

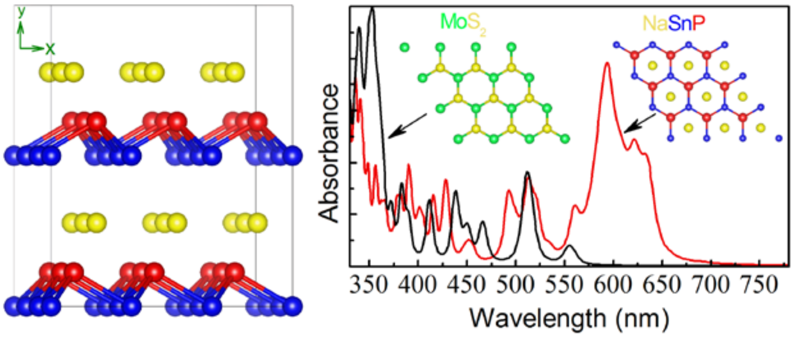

Fig. 1 Crystal structure of NaSnP; the light absorption spectra of NaSnP (red line) and MoS2 monolayers (black line)

In this work, density functional theory (DFT) calculations were performed to study the structural, mechanical, electrical, optical properties, and strain effects in single-layer sodium phosphidostannate-(II) (NaSnP).[1] We find the exfoliation of single-layer NaSnP from bulk form is highly feasible because the cleavage energy is comparable to graphite and MoS2. In addition, the breaking strain of the NaSnP monolayer is comparable to other widely studied 2D materials, indicating excellent mechanical flexibility of 2D NaSnP. Using the hybrid functional method, the calculated band gap of single-layer NaSnP is close to the ideal band gap of solar cell materials (1.5 eV), demonstrating great potential in future photovoltaic application. Furthermore, strain effect study shows that a moderate compression (2%) can trigger indirect-to-direct gap transition, which would enhance the ability of light absorption for the NaSnP monolayer. With sufficient compression (8%), the single-layer NaSnP can be tuned from semiconductor to metal, suggesting great applications in nanoelectronic devices based on strain engineering techniques.

Eisenmann, B. and U. Rößler, Crystal structure of sodium phosphidostaimate(II), NaSnP, Zeitschrift für Kristallographie - New Crystal Structures. 1998, 213, 28−28.

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Analysis of In2S3 Buffer Layer Properties Effects on a CIGS Solar Cell Performance Using SCAPS

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A simulation study is used to investigate the effect of Indium Sulfide buffer layer geometry and its electro-optical properties on the Copper Indium-Gallium-Diselenide (CIGS) solar cell performance. The energy band gap of In2S3 can vary within the range of 2.1 eV to 2.9 eV due to the process temperature and the oxygen content in the respective deposited film. The variation of the band gap (E_g) is related to changes in absorption coefficient (α) and is associated with the variation of electron affinity (x_e) [1].

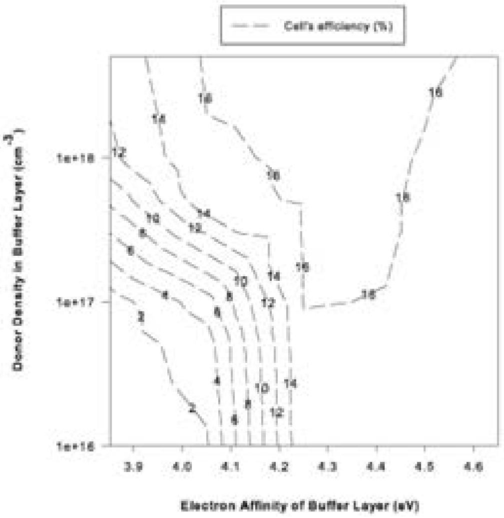

Figure 1. Contour plot of cell efficiency variation versus buffer band gap and donor density.

The energy band gap of In2S3 and its estimated functional relation with the Indium Sulfide electron affinity is extracted using available valid data [2-4] and is shown by the equation (1):

$$E_g = 6.75 - x_e$$

In this simulation the In2S3 donor density was varied in the range of 1E+16 cm-3 and 5E+18 cm-3. The buffer layer's thickness were changed within the range of 0.03 µm - 1 µm. The simulation results obtained with SCAPS show the cell a with thinner In2S3 buffer layer represents higher performance and accordingly the thickness of less than 0.1 µm is proposed as the optimum range for the buffer layer. As a result, the optimum electron affinity and donor density of the buffer layer is found to be

4.25 + 0.2 eV and over 1.0E+17 cm-3

respectively.

References:

[1] S. M. Sze and K. K. Ng, Physics of semiconductor devices: Wiley. com, 2006.

[2] N. Barreau, S. Marsillac, D. Albertini, and J. Bernede, "Structural, optical and electrical properties of β-In2S3-3xO3x thin films obtained by PVD," Thin Solid Films, vol. 403, pp. 331-334, 2002.

[3] N. Barreau, S. Marsillac, J. C. Bernède, and L. Assmann, "Evolution of the band structure of β-In2S3−3xO3x buffer layer with its oxygen content," Journal of Applied Physics, vol. 93, p. 5456, 2003.

[4] R. Robles, N. Barreau, A. Vega, S. Marsillac, J. Bernede, and A. Mokrani, "Optical properties of large band gap β-In2S3− 3xO3x compounds obtained by physical vapour deposition," Optical Materials, vol. 27, pp. 647-653, 2005.

Phosphorene: Anisotropic Electronic/transport properties of a unique 2D material

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Phosphorene, the single- or few-layer form of black phosphorus, was recently rediscovered as a two-dimensional layered material holding great promise for applications in electronics and optoelectronics [1]. Research into its fundamental properties and device applications has since seen exponential growth.

Here we study the adsorption of CO, CO2, NH3, NO, and NO2 gas molecules on a monolayer phosphorene [2]. Our results predict superior sensing performance of phosphorene that rivals or even surpasses that of other 2D materials such as graphene and MoS2. We determine the optimal adsorption positions of these molecules on the phosphorene and identify molecular doping, that is, charge transfer between the molecules and phosphorene, as the driving mechanism for the high adsorption strength. The transport features show large (1–2 orders of magnitude) anisotropy along different directions, which is consistent with the anisotropic electronic band structure of phosphorene. Remarkably, the I–V relation exhibits distinct responses with a marked change of the I–V relation along either the armchair or the zigzag directions depending on the type of molecules. Such selectivity and sensitivity to adsorption makes phosphorene a superior gas sensor that promises wide-ranging applications.

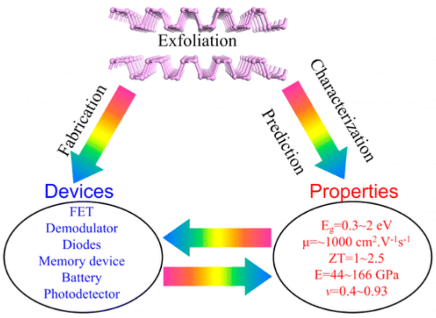

Figure 4 Graphene crystal and application

Meanwhile we unveil a new, highly anisotropic ripple pattern in phosphorene [3], where compression-induced ripple deformation occurs only along the zigzag direction in the strain range up to 10%, but not the armchair direction. This direction-selective ripple deformation mode in phosphorene stems from its puckered structure with coupled hinge-like bonding configurations and the resulting anisotropic Poisson ratio. We also construct an analytical model using classical elasticity theory for ripple deformation in phosphorene under arbitrary strain. The present results offer new insights into the mechanisms governing the structural and electronic properties of phosphorene crucial to its device applications.

1. Kou, L. K., Chen, C. F., Smith, S. Phosphorene: Fabrication, Properties, and Applications. J. Phy. Chem. Lett, 2015. 6(14): p. 2794-2805.
2. Kou, L. K., Chen, C. F., Smith, S. Phosphorene: Fabrication, Properties, and Applications. J. Phy. Chem. Lett, 2014. 5(15): p. 2675-2681.
3. Kou, L. K., Chen, C. F., Smith, S. Phosphorene: Fabrication, Properties, and Applications. J. Phy. Chem. Lett, 2015. 6(9): p. 1509-1513.

Bi donors in silicon for clock transitions and implant precision

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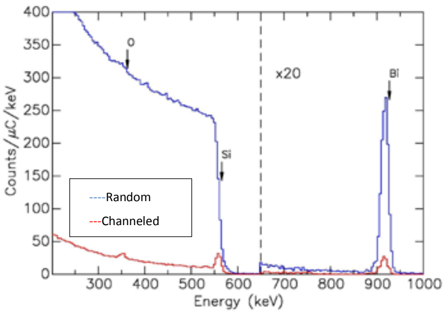
The unusual attributes of the bismuth atom include a large nuclear spin of 9/2 and hyperfine energy levels that have attractive attributes including clock transitions [1,2]. Such transitions are very stable against perturbations from external electromagnetic fields and therefore have significantly long lifetimes for the storage of quantum information. This is especially important for bismuth atoms incorporated into an engineered nano-device that exploits the clock transition because of the intrinsically noisy environment associated with gate oxides and metal gates necessary for spin control. Bismuth atoms may be implanted into silicon where they can become electrically active n-type donors. Amongst all n-type donors in Si, the greatest placement precision by implantation can be achieved with bismuth. The availability of a clock transition and this low straggling is a unique combination making bismuth very attractive for the fabrication of arrays of single atoms [3] and ultra-scaled nanofabricated devices for various quantum technologies.

As the first step to harness the attributes of bismuth for these technologies we have investigated the implantation and annealing of bismuth in natural silicon [4]. Measurements with ion channeling have revealed that the implanted bismuth atoms have a lattice substitution of greater than 90% following the optimum



Rutherford backscattering <100> channeling measurements of the implanted Bi lattice substitution fraction (1 MeV He, detector angle 170°)

annealing strategy of 700°C for 10 minutes in forming gas. We review the next steps for this promising materials system to investigate the spin lifetime in bismuth implanted silicon MOSFETs.

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References:

1. S. Rogge, M.J. Sellars, *Atomic clocks in the solid state*, Nature Nanotechnolopgy 8, 544 (2013)
2. G. Wolfowicz, A.M. Tyryshkin, R.E. George, H. Riemann, N.V. Abrosimov, P. Becker, H-J. Pohl, M.L.W. Thewalt, S.A. Lyon, J.J.L. Morton, *Atomic clock transitions in silicon-based spin qubits,* Nature Nanotechnology 8, 561–564 (2013)
3. J.A. van Donkelaar, C Yang, ADC Alves, et al., *Single atom devices by ion implantation*, Journal of Physics: Condensed Matter, 27, 154204 (2015)
4. J. P. de Souza and P. F. P. Fichtner, *Electrical activation of bismuth implanted into silicon by rapid thermal annealing and kinetics of defects,* Journal of Applied Physics 74, 119 (1993)

Encapsulating Quantum Dots into ZnO Nano/Microrods for Advanced photonics Applications

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Colloidal quantum dots (QDs) are promising for new-generation light-emitting devices and lasers[1]. We encapsulate QDs with various emission colours into single-crystal ZnO nanorods or microrods by exploiting the crystal growth of ZnO in chemical bath. The hexagonal structure of ZnO crystals can act as optical cavity [2] and the QDs are light sources when stimulated by an external laser. Therefore either Fabry-Perot (FP) type or whispering-gallery mode (WGM) resonances are anticipated to occur [3]. Unlike conventional semiconductor lasers that have fixed emission wavelengths and limited choices for emitting colour, the nano/microrod laser with QDs as emitters have a number of options for wavelength selection. For example, multi-color emissions from a single nano/microrod can be achieved by loading different types of QDs into the same nano/microrod cavity [4]. We propose to develop new kind of LEDs by using QDs loaded n-type ZnO nanorods grown on p-type GaN substrates, in order to exploit the UV

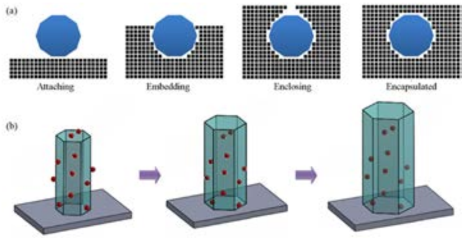

Fig 1 (a) Illustration of the encapsulation process of a surface-attached quantum dots into the growing crystal. (b) Encapsulation of QDs into a ZnO nanorod by regrowing the nanorod [4].

emission of ZnO to excite the photoluminescence of QDs. Our study will not only lead to the development of color-tunable lighting devices and lasers, but will open the way to a plethora of applications, beyond those of conventional semiconductor lighting devices.

[1] D. Bera, L. Qian, T. K. Tseng, et al. Quantum dots and their multimodal applications: a review. Materials, 2010, 3, 2260-2345.

[2] Jinzhang Liu, Nunzio Motta. The nanonail flower–toward tailored ZnO nanostructures. Materials Today, Vol. 17, 307. July 2014.

[3] T. Nobis, M. Grundmann. Low-order optical whispering gallery modes in hexagonal nanocavities. Physical Review A. 2005, 72, 063806.

[4] Liu, J., M. Notarianni, L. Rintoul, and N. Motta, Encapsulation of nanoparticles into single-crystal ZnO nanorods and microrods. Beilstein Journal of Nanotechnology, 2014. 5: p. 485-493.

Structural, Electrical, Mechanical and Optical Properties of BiI3 monolayer

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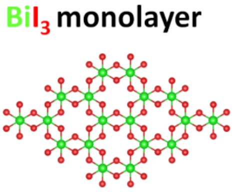
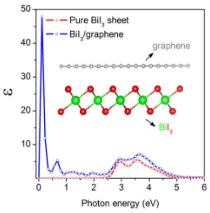
Since the discovery of graphene and its excellent electronic/mechanical properties, tremendous research efforts have been focusing on searching new two-dimensional (2D) materials including hexagonal boron nitride, transition metal dichalcogenides and many others. These 2D materials are bringing revolutions to numerous advanced applications due to their unique and fascinating physical and chemical properties. Up to now, a diverse range of intriguing properties in 2D materials have been revealed, highlighting the potential use for important applications in energy, photonics and nanoelectronics. However, the practical applications based on 2D materials are very limited because they suffer from serious bandgap hurdles, i.e., the lack of obvious gap in graphene [1] and too large gap in boron nitride. [2] Single layer metal di-chalcogenide such as MoS_2 possess an appropriate bandgap, [3] but are strongly effected by metal contacts, charged impurities, and structural defect. Therefore, the search for new types of 2D structures is of paramount importance for the fabrication of next generation nanodevices.





By using density functional theory (DFT) methods, here we investigate in detail the structural, electronic, mechanical and optical properties in single layer bismuth iodide (BiI_3) nanosheet. Monolayer BiI_3 is first confirmed to be dynamically stable by the phonon spectrum. The cleavage energy (Ecl) and strength of BiI_3 are comparable to the experimentally values of graphite, which indicates the exfoliation of BiI_3 is highly feasible. The monolayer BiI3 is an indirect semiconductor with a gap around 1.5 eV with spin orbit coupling (SOC). Furthermore, the band gap of monolayer BiI_3 nanosheet can be modulated by biaxial strain. Most interestingly, interfacing electrically active graphene with monolayer BiI_3 nanosheet shows a significant red shift of absorption edge up to 2.0 eV compared to that in pure monolayer BiI_3 nanosheet, highlighting great potential applications in photonics and photovoltaic solar cells.

1. Zhou, S.; Gweon, G.-H.; Fedorov, A.; First, P.; De Heer, W.; Lee, D.-H.; Guinea, F.; Neto, A. C.; Lanzara, A., Substrate-Induced Bandgap Opening in Epitaxial Graphene. *Nature materials* **2007**, *6*, 770-775.
2. Tang, Q.; Zhou, Z.; Chen, Z., Molecular Charge Transfer: A Simple and Effective Route to Engineer the Band Structures of Bn Nanosheets and Nanoribbons. *The Journal of Physical Chemistry C* **2011**, *115*, 18531-18537.
3. Wang, Q. H.; Kalantar-Zadeh, K.; Kis, A.; Coleman, J. N.; Strano, M. S., Electronics and Optoelectronics of Two-Dimensional Transition Metal Dichalcogenides. *Nat Nano* **2012**, *7*, 699-712.

Ultra-Sensitive Photodetectors by Hierarchical Nanoparticles Network

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Ultraviolet (UV) photodetector have a wide range of application in water sterilization, military, flame detection, optical communication, early missile launch detection and astronomy.[1-3] Metal-oxide semiconductors such as ZnO are excellent materials for the fabrication of solid-state photodetectors.

Zinc oxide is a promising transparent conductive oxide with great luminescence and electrical properties due to its wide band-gap (3.37 eV at 300 K) and large excitonic binding energy (about 60meV).[1,4] Recently, a variety of photodetector generation have been studied that are suitable to produce a good-quality ZnO films fabricated by the well-known techniques such as RF magnetron sputtering,[5] sol-gel,[6,7] Chemical vapor deposition (CVD)[8] and pulsed laser deposition.[9] Previous researches[3] demonstrated a novel flame transport synthesis for in situ integration of the ZnO nanostructure-based UV detectors on a substrate during a growth process. Fabricated photo-detector devices exhibited a high current ratio IUV/Idark ≈ 4.5 × 103 at 2.4 V which was significantly higher compared to the previous researches. In another approach[10], a high-performance transparent photodetector fabricated by electrospun ZnO-SnO2 nanofibers film with a good Ohmic contact and IUV/Idark of 4.6 × 103.

Here, we use one-step flame spray deposition method as a cheap, simple and fast method to produce fully transparent highly porous nanoparticle films as alterative morphology for the assembly of UV photodetectors. The synthesis process is simple and could be easily scaled up. Films were self-assembled by direct aerosol deposition of ZnO nanoparticles on interdigitated glass substrates. The effect of precursor concentration (particle size) on photodetector efficiency was investigated here. We show that the device is inherently visible-blind and its performance in terms of IUV/Idark is significantly higher (13.6 × 104) compared to the previous researches.

1. J. Sun, F.-J. Liu, H.-Q. Huang, J.-W. Zhao, Z.-F. Hu, X.-Q. Zhang, Y.-S. Wang, Applied Surface Science 2010, 257, 921.
2. Y. Jin, J. Wang, B. Sun, J. C. Blakesley, N. C. Greenham, Nano Letters 2008, 8, 1649.
3. D. Gedamu, I. Paulowicz, S. Kaps, O. Lupan, S. Wille, G. Haidarschin, Y. K. Mishra, R. Adelung, Advanced Materials 2014, 26, 1541.
4. S. M. Hatch, J. Briscoe, S. Dunn, Advanced Materials 2013, 25, 867.
5. R. Liu, D. Jiang, Q. Duan, L. Sun, C. Tian, Q. Liang, S. Gao, J. Qin, Applied Physics Letters 2014, 105.
6. M. H. Mamat, Z. Khusaimi, M. Z. Musa, M. Z. Sahdan, M. Rusop, Materials Letters 2010, 64, 1211.
7. S.-E. Ahn, H. J. Ji, K. Kim, G. T. Kim, C. H. Bae, S. M. Park, Y.-K. Kim, J. S. Ha, Applied Physics Letters 2007, 90.
8. J. Liu, R. Lu, G. Xu, J. Wu, P. Thapa, D. Moore, Advanced Functional Materials 2013, 23, 4941.
9. N. Hernandez-Como, S. Moreno, I. Mejia, M. A. Quevedo-Lopez, Semiconductor Science and Technology 2014, 29, 085008.
10. W. Tian, T. Zhai, C. Zhang, S.-L. Li, X. Wang, F. Liu, D. Liu, X. Cai, K. Tsukagoshi, D. Golberg, Y. Bando, Advanced Materials 2013, 25, 4625.

Room temperature gas sensing properties of ultrathin carbon nanotube films by surfactant-free dip coating

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Carbon nanotubes (CNTs) based sensors have been intensively studied in the past years due to their attractive properties including high sensitivity, room temperature operation, and very low detection limit [1-2].

A fabrication method that accurately controls CNT film morphology is crucial for the development of reliable and high sensing performance chemiresistors. Moreover, this technique must be low-cost and scalable for high volume production in order to ease their integration into mass production devices . Many CNT film fabrication techniques are either not scalable or rely on the use of CNT dispersions obtained using surfactants, however these are known to be problematic because of the difficulty in removing the surfactants from the CNTs once the film is formed. Chlorosulfonic acid has been shown to be the only true solvent for CNTs [3] and has been successfully used to produce CNT surfactant-free thin films by scalable dip coating [4].

In this presentation, we report the fabrication of highly sensitive conductometric devices to NO_2 and NH_3 gases at room temperature using a sensing layer of dip coated CNT films made from chlorosulfonic acid solutions. In order to get a deeper understanding of the sensing mechanism, we developed ultrathin CNT films with different thicknesses and compared their sensing performances. We found good sensing performances to concentrations as low as 1 ppm for NO_2 and 7 ppm for NH_3. Continuous *in-situ* UV irradiation was found not only to accelerate gas desorption but also to increase the gas response.

1. Kong, J.; Franklin, N. R.; Zhou, C.; Chapline, M. G.; Peng, S.; Cho, K.; Dai, H., *Science* **2000**, *287*, 622-625.
2. De Volder, M. F. L.; Tawfick, S. H.; Baughman, R. H.; Hart, A. J., *Science* **2013**, *339*, 535-539.
3. Parra-Vasquez, A. N. G., et al., *ACS Nano* **2010**, *4*, 3969-3978.
4. Mirri, F.; Ma, A. W. K.; Hsu, T. T.; Behabtu, N.; Eichmann, S. L.; Young, C. C.; Tsentalovich, D. E.; Pasquali, M., *ACS Nano* **2012**, *6*, 9737-9744.

Photoluminescence properties of individual ZnO nanowire

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As wide-bandgap semiconductor, ZnO is a very attractive candidate for blue and UV optoelectronics [1]. In this work we investigated photoluminescence (PL) properties of individual ZnO nanowire (NW), prepared by evaporation condensation technique, then dispersed in isopropanol and transferred on different substrates (as SiO_2, SiO_2/Si p-doped, p-GaN, or p-SiC).

The choice of a single nanowire - instead of mesh of nanowires with a wide diameter distribution - allows to better understand the properties of the material and to investigate the PL emission properties as a function of the nanowire dimensions.

PL maps of single nanowires show that as the diameter of the wire decreases, a shift in the near band edge (NBE) PL is observed, in accordance with Ref. [2].

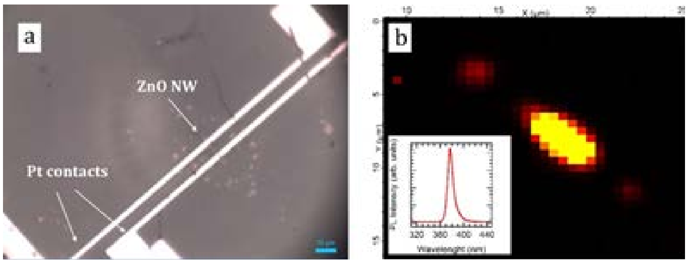

Figure 5: (a) Micro-optical image of individual ZnO nanowire across Pt electrical contacts. (b) NBE peak (in the inset) PL map of the ZnO NW (the shadow regions at the ends of the PL map correspond to the Pt contacts).

Temperature dependent PL spectra (from RT to 77 K) of ZnO single NW has been carried out in order to assign peaks corresponding to free exciton (FX), donor bound exciton (DX) and LO-assisted FX [3] and to reach insight on the mechanism responsible for PL emission of the nanowires as the diameter changes.

Pt contacts has been deposited by electron beam lithography (EBL) on the single ZnO NW, as shown in Fig 1a. This allows us to obtain PL information as function of the current flowing in the NW or, in FET configuration, as function of gate voltage applied.
Finally, the deposition of n-type ZnO NWs on different substrates, in particular on p-type substrates, allows to observe heterojunction effects at the nanoscale level which play a crucial role in the perspective of ZnO based nano-optoelectronic devices production.

1. J. Bao, M.A. Zimmler, F. Capasso, Z. Wang, and Z.F. Ren, *Broadband ZnO single-nanowire light-emitting diode.* Nano Letters, 2006. **6**: p. 1719-1722.
2. X. Zhang, D. Liu, L. Zhang, W. Li, M. Gao, W. Ma, Y. Ren, Q. Zeng, Z. Niu, W. Zhou, and S. Xie, *Synthesis of large-scale periodic ZnO nanorod arrays and its blue-shift of UV luminescence*. J. Mater. Chem., 2009. **19**: p. 962-969.
3. .W. Hamby, D.A. Lucca, M.J. Klopfstein, and G. Cantwell, *Temperature dependent exciton photoluminescence of bulk ZnO*. J. of applied Physics, 2003. **93**: p. 3214-3217.

Prediction of a large-gap Quantum Spin Hall Insulator in 3D Thorium Oxychalcogenides and 2D Diamond-like GaBi Bilayer

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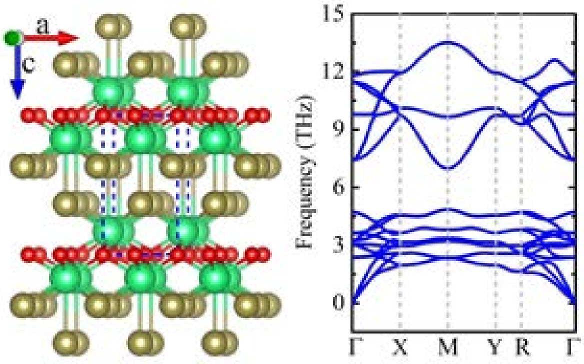

Figure 1 Structure and Phonon spectrum

Figure 6 Grahene crystal

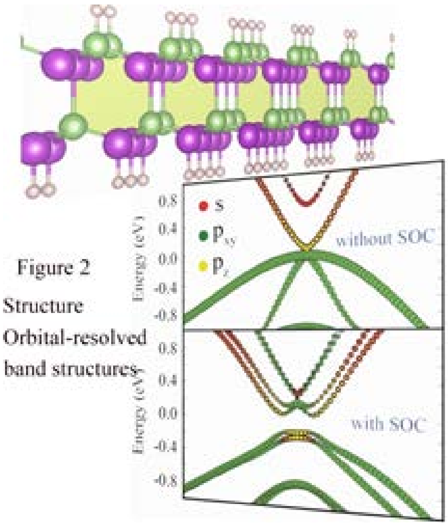

Figure 2 Structure Orbital-resolved band structures

Three dimensional (3D) Topological Insulators (TIs), whose variants can host magnetism and superconductivity have generated widespread research activity in condensed-matter and materials-physics communities [1]. The search for new and realistic 3D TIs has greatly benefited from the fruitful interplay between topological band theory and realistic band structure calculations. we for the first time predict that the experimentally-realized 3D thorium oxychalcogenide (ThOTe) is dynamically stable and can realize novel quantum spin Hall (QSH) phase, with a nontrivial band gap of 0.154 eV, suggesting that the 3D ThOTe lattice could be a versatile platform for hosting nontrivial topological states with potential application in 3D spintronics and computer technology.

Meanwhile, it was widely accepted that two dimensional (2D) TIs possess unique advantages over 3D TIs because all the scatterings of electrons are completely forbidden in 2D materials. This leads to dissipationless charge or spin current carried by edge states, and the charge carriers can be also easily controlled by gating [2]. Using density functional theory (DFT), we demonstrated that the hydrogenated GaBi bilayers (HGaBi) is a stable topological insulator with a large nontrivial band gap of 0.320 eV based on the state-of-the-art hybrid functional method, which is implementable for achieving QSH states at room temperature.

1. Hsieh, D., *et al.* Observation of unconventional quantum spin textures in topological insulators. Science, 2009. **323**: P. 919-922.
2. Si, C., *et al.* Functionalized germanene as a prototype of large-gap two-dimensional topological insulators. Physical Review B, 2014. **89**: P. 115429.

Mechanical behavior of Graphene under impact loading

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Carbonaceous materials like CNT rope and CNT wire have been adopted in antiballistic application due to its high strength, light weight and excellent energy absorption capacity (Atkinson et al., 2007; De Volder, Tawfick, Baughman, & Hart, 2013; Gardner, Peoples, & Rosenberger, 2011; Mylvaganam & Zhang, 2007). Graphene, a honeycomb structure carbon allotrope, has been reported with exceptional in-planar yield stress and Young's modulus at quasi-static conditions; however its behavior under extreme dynamic conditions is rarely discussed in literature. Basing on the large-scale molecular dynamics simulation, the mechanical behavior of the single layer graphene and the multi-layer graphene over a range of thicknesses is investigated under the impact loadings achieved by a diamond bullet with speed varying between 500 and 3500ms-1. The stress and strain distribution pattern of graphene upon the impact loading is discussed and the specific penetration energies for the single layer and multi-layer graphene are calculated. In addition, penetration features of different layers of graphene are also presented. It is expected that this study will establish the understanding of the mechanical behavior of the graphene and guide its antiballistic application in the near future.

Atkinson, K. R., Hawkins, S. C., Huynh, C., Skourtis, C., Dai, J., Zhang, M., . . . Aliev, A. E. (2007). Multifunctional carbon nanotube yarns and transparent sheets: fabrication, properties, and applications. Physica B: Condensed Matter, 394(2), 339-343.

De Volder, M. F., Tawfick, S. H., Baughman, R. H., & Hart, A. J. (2013). Carbon nanotubes: present and future commercial applications. Science, 339(6119), 535-539.

Gardner, S. H., Peoples, J. R., & Rosenberger, B. T. (Singer-songwriters). (2011). Ballistic fabrics with improved antiballistic properties. On: Google Patents.

Mylvaganam, K., & Zhang, L. (2007). Ballistic resistance capacity of carbon nanotubes. Nanotechnology, 18(47), 475701.

Application of Polymers in Carbon Nanotube Silicon Heterojunction Solar Cells

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Recently, researchers are starting to combine polymer materials with carbon nanotube silicon heterojunction (NHS) to enhance the performance of devices. Based on different positions of the polymer layers added to NSH cells, there are 2 main kinds, a top antireflection layer or an interlayer, as shown in figure 1. The antireflection layer is utilized to decrease the reflection of photon energy from silicon surface which can reflect over 30% of light [1] [2]. The interlayer can enhance the depletion region due to better conformal surface covering by polymer layer [3]. Specifically, for each polymer layer, 3 types of polymer (table 1) have been used and the effect of various compositions in the 2 layers on NSH device performance has been studied.

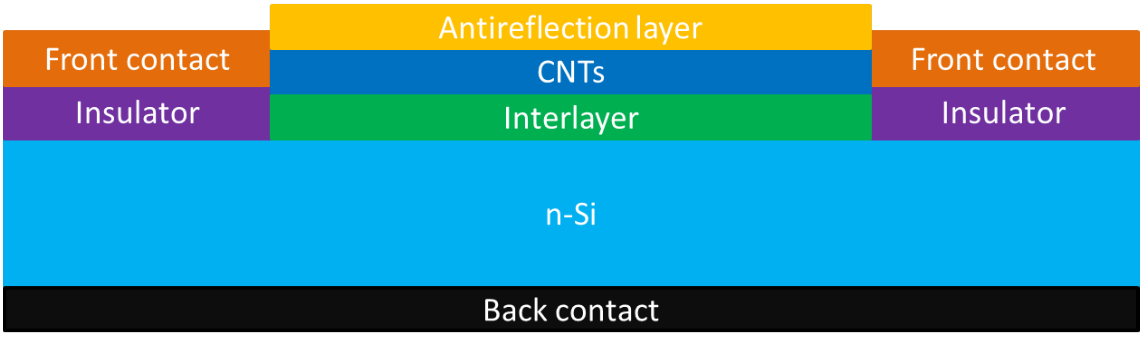

Figure 1: Schematic of NSH device structure combined with polymer layer

The results showed that antireflection layer could improve the performance effectively while the effect of interlayer was dependent on the type of the layer applied. A particular solar cell with efficiency about 8.66% was fabricated by adding PS (75 nm) as the antireflection layer on top of CNTs film, and PEDOT:PSS as the interlayer.

Antireflection layer	Polydimethylsiloxane (PDMS)
	Poly(methyl methacrylate) (PMMA)
	Polystyrene (PS)
Interlayer	Polyaniline (PANI)
	Poly(3-hexylthiophene-2,5-diyl) (P3HT)
	Poly(3,4-ethylenedioxythiophene): poly(styrene sulfonate) (PEDOT:PSS)

Table 1: Details of polymer layer for both antireflection and interlayer

References:

1. Jia, Y., Li, P., Gui, X., Wei, J., Wang, K., Zhu, H., Wu, D., Zhang, L., Cao, A. & Xu, Y. 2011. *Applied Physics Letters*, **98**, 133115.
2. Tune, D. D., Flavel, B. S., Quinton, J. S., Ellis, A. V. & Shapter, J. G. 2013. *ChemSusChem,* 6, 320-7.
3. Li, R., Di, J., Yong, Z., Sun, B. & Li, Q. 2014. *Journal of Materials Chemistry A,* **2**, 4140.

The current status of CZTS Thin Film Solar Cells in Photovoltaic

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Solar energy, as a clean and sustainable energy type, has been developed and applied in the production of electric powers for decades. The importance of using solar energy originates from the environment concern and the unrenewable of the traditional fossil fuels. With the increasingly demanding of energy and the environment protection requirement, low cost and environment-friendly energy production are desired to replace the traditional power supply.

Photovoltaic (PV) technologies have been developed to produce electric power. Si-based solar cells, the first generation PV, have been commercialised. However, in order to enhance the photovoltaic conversion efficiency (PCE), the fabrication processes are more and more complex, which lead to the rising cost of the solar electricity. In addition, the PCE of Si- based solar cells is very close to its efficiency limit predicted by Shockley-Quisser model [1]. The second generation PV devices based on thin film solar cells such as CIGS and CdTe has also started to be produced in large scale as their efficiency already surpasses 20% [2], which is crucial for commercialization. However, the component elements used in CIGS and CdTe such as In, Ga, Cd are not abundant in the earth crust and/or toxic to the environment.

Cu2ZnSnS4 (CZTS) which has the similar structure and properties with CIGS is only constructed by using earth-abundant and non-toxic materials. However, the currently highest PCE of CZTS thin film solar cells is 12.6% [3] and the power loss mechanism in the solar cells is still unclear yet. Lots of methods have been used to fabricate CZTS including solution-based and vacuum-based [4]. Several key issues that need to be solved will be discussed in order to enhance the quality of CZTS and further improve the device performance.

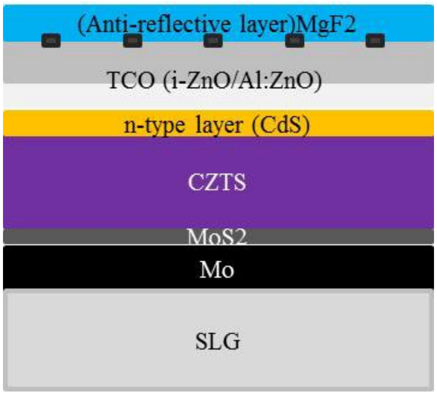

Figure 1 Typical CZTS solar cells structure

William Shockley and Hans J. Queisser, J. Appl. Phys. 1961, 32: p510

Martin A. Green, Keith Emery, Yoshihiro Hishikawa, Wilhelm Warta and Ewan D.Dunlop, Prog. Photovolt: Res. Appl. 2015, 23: p1–9

Wei Wang , Mark T. Winkler , Oki Gunawan , Tayfun Gokmen , Teodor K. Todorov , Yu Zhu and David B. Mitzi, Adv. Energy Mater. 2014, 4: p1301465

HongxiaWang, International Journal of Photoenergy 2011, 2011: p801292

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Workshop Keynote/Invited Speakers Abstracts

Access and control over quantum states in the solid state

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Semiconductor nano devices whose operation derives from the bound states of individual dopants have received considerable attention because of the promise for new functionalities in quantum electronics [1]. Silicon offers a particularly interesting platform for single dopants because when isotopically purified, silicon acts as a “semiconductor vacuum” for spin, giving it extraordinary coherence. Although more difficult in silicon, optical control of single qubits is very attractive since it allows for precision quantum control with ultrahigh spectral resolution, and could enable long distance communication.

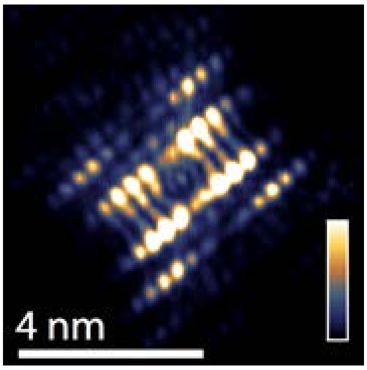

Figure 7 Buried P in Si.

This talk will discuss optical addressing and electrical detection of individual erbium dopants with exceptionally narrow line width. The hyperfine coupling to the Er nucleus is clearly resolved, which paves the way to single shot readout of the nuclear spin, and is the first step towards an optical interface to dopants in silicon [2]. Furthermore, spatially resolved tunneling experiments performed by cryogenic scanning tunneling spectroscopy will also be discussed [3]. They reveal the spectrum and wavefunction of both single dopants, see Fig. 1, and exchange-coupled dopant molecules. Donors up to 5 nm below a silicon surface are measured, and exhibited quantum interference processes reflecting the valley degrees of freedom inherited from the silicon “semiconductor vacuum”. Finally, exchange-coupled solid-state molecules were studied. The signature of quantum correlations and entanglement were detected by spatially resolved local tunneling spectroscopy experiments in the single-hole tunneling regime. With increasing bond distance, evidence was found for a crossover from an uncorrelated state, to a correlated state.

Finally, we will discuss spatially resolved spectroscopy of buried dopant structures fabricated with the STM spanning from atoms to devices.

1. Zwangenburg, F.A., Silicon quantum electronics. Reviews of Modern Physics, 2013. 85(3): p. 961.

2. Yin, C., Optical addressing of an individual erbium ion in silicon. Nature, 2013. 497 (7447): p. 91.
3. Salfi, J., Spatially resolving valley quantum interference of a donor in silicon. Nature Materials, 2014. 13 (6): p. 605

Professor Sven Rogge

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Sven Rogge received his PhD in Physics from Stanford University (USA) in 1997. Thereafter he moved to the Delft University of Technology in the Netherlands and become a faculty member in 2003. During his time in Delft he was awarded a fellowship from the Royal Netherlands Academy of Arts and Sciences (KNAW) in 2000. In 2010 was awarded an Australian Research Council (ARC) Future Fellowship and moved to the University of New South Wales (UNSW, Australia) in 2011. At UNSW he is a distinguished Professor and Head of the School of Physics and a Program Manager at the ARC Centre of Excellence for Quantum Computer and Communication Technology.

Controlling electrons one at a time in Silicon ultra-scaled devices

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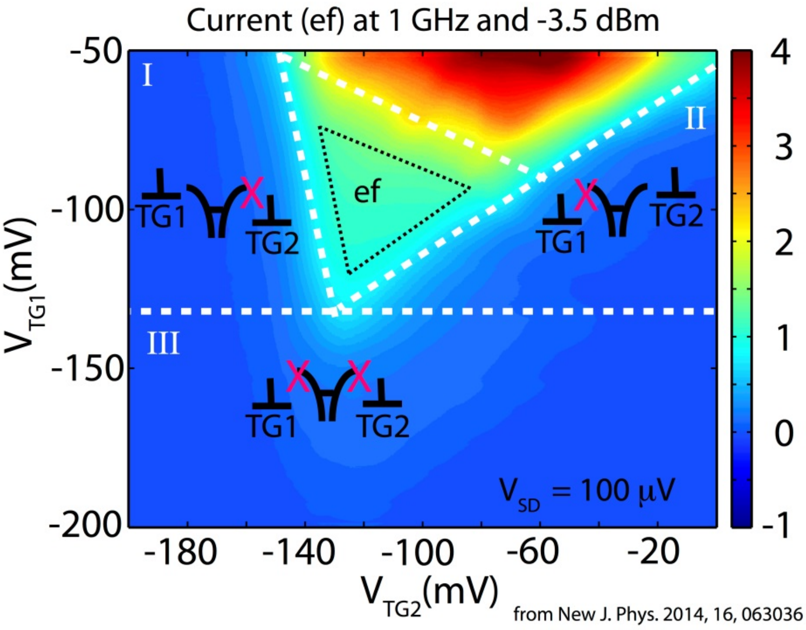
The strong focus on quantized electron pump (QEP) is justified by their ability to generate currents in which capture and emission processes can be controlled at the single electron level [1-4]. This can be obtained by taking advantage of Coulomb blockade (CB) effects [1-4]. By using a single dopant atom quantised electrons pump (SDA-QEP), a new kind of QEP has been recently demonstrated [1,2]. The characteristics of the SDA-QEP were found to be quite different from the more conventional quantum dot charge pumps (QD-QEP's) [3]. This difference originates from the intrinsic dissimilarity in the confinement potential that traps the electrons [1-3]. In my talk, I will discuss a new SDA-QEP model that describes the behaviour in terms of frequency, power and the position of the dopant in the channel. Other kind of silicon devices recently fabricated and studied will also be discussed in my talk.



from New J. Phys. 2014, 16, 063036

1. Tettamanzi, G. C. and Wacquez R. and Rogge S., New J. Phys. 2014, 16, 063036.
2. Tettamanzi, G. C., van der Heijden J. and Rogge S., IEEE Proc. of the 2014 COMMAD, pp 298-300.
3. Rossi A. and Tanttu T. and Tan K. Y. and Iisakka I. and Zhao R. and Chan K. W. and Tettamanzi G. C. and Rogge S. and Dzurak A. S. and Mottonen M., Nano Letters 2014, 14, 3405.
4. Pothier H et al 1992 Europhys. Lett., 17 249.

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After graduating with a Master Degree in Solid State Physics at the University of Rome, La Sapienza and successively with a PhD Degree in Applied Superconductivity at the University of Melbourne, I moved to the Kavli Institute of Nano-Science in Delft as Foundation for Fundamental Research on Matter (FOM) research fellow within the Photronic Group. From 2012 and 2014, I was also the holder of a ARC DECRA fellowship. Since the DECRA award in late 2011, I have established independent research in Silicon-based Quantum Metrology. In addition, since the UNSW GOLDSTAR award in 2012, I have extended this effort and opened up new lines of research focusing on novel hybrid Superconductor-Semiconductor Single Atom Transistor devices and on two-dimensional transistors. In my career I have established unique skills in the physics of ultra-small CMOS devices, on Applied Superconductivity, on Ultra Low Noise and on Ultra Low Temperature Techniques

Measuring spin states and tunnel couplings of electrons in atomic precision Si:P devices.

Matthew House

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The seminal proposal for a solid state quantum computer by Kane in 1998 called for quantum information to be stored in the nuclear spin states of 31P atoms hosted in a silicon crystal and transferred to the singlet-triplet spin states of two electrons for manipulation and readout [1]. Since then advancements in scanning tunnelling microscope lithography have progressed to the point where we can place individual P donors in Si with atomic-scale precision [2]. Among the remaining challenges to constructing a quantum computer using this technology are an understanding of the device geometry needed to achieve good tunnel couplings between donors, and the ability to engineer charge sensing in complex devices at such small length scales. In recent work we use radio frequency reflectometry to measure the singlet and triplet states of a few-donor Si:P silicon double quantum dot [3]. We demonstrate the utility of analyzing both the amplitude and phase of the reflected rf signal for measuring tunnel couplings between the dots and their respective leads, which on one dot we find increases from 150 MHz to 22 GHz as the number of electrons is changed from 1 to 4. We extract an accurate measure of the tunnel coupling of 47±5 □eV between the two dots, separated by 11.5 nm, and observed that the exchange coupling at this transition is tunable by more than two orders of magnitude using monolayer, in-plane gates defined by P doping. We measured a singlet-triplet relaxation time of 60 ns and show that this fast relaxation rate is not inherent to the spin system but to be limited by strong tunnel coupling to electronic states in the leads. These results provide a comprehensive measurement of tunnel coupling and exchange in donor-based devices and represent important steps towards implementing the Kane model of quantum computation using phosphorus nuclear spins in silicon [3]

Dr Matthew House

The UNSW, Sydney, Australia

Dr. House is currently a postdoctoral research fellow in Michelle Simmons' group at the Centre for Quantum Computation and Communcation Technology, UNSW Australia, where he studies the fabrication, operation, and physics of silicon devices doped with phosphorus by scanning tunnelling microscope lithography. He received his Ph. D. in 2012 from UCLA, where he studied electron spin physics for quantum computing applications in silicon MOSFET devices.

Direct imaging of straggled ions for top-down fabrication of Si:P qubits in nano-scale devices using atom probe tomography

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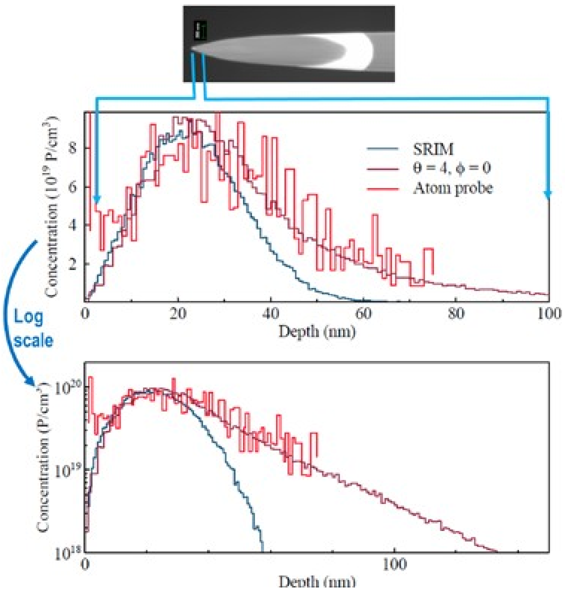
Single 31P ions can be deterministically implanted (“top-down”) into isotopically pure 28Si substrates to build devices in which information can be encoded in the quantum states of the 31P donor electron spin or nuclear spin. In the case of the nuclear spin, coherent states can be sustained with remarkably long T2 times in excess of 30 s [1]. Exploiting these results to build a large-scale device based on detemrinsiitic single atom nanotechnology requires careful architecture design consistent with the precision limitations of the deterministic implantation method.



High depth reolution atom probe profile of 14 keV ^{31}P implanted into Si: Work by J. Douglas, Oxford, B. Johnson, Melbourne.

Donor atom positioning no deeper than 20 nm below the gate oxide and ion straggling constrains the implantation energy to below 14 keV and preferably below 10 keV. Models for the straggling process, for example the Stopping and Range of Ions in Matter (SRIM) and crystal- Transport of Ions In Matter (TRIM), allow for constraints imposed by various effects to be evaluated. We have employed Atom Probe Tomography, to facilitate the measurement of lowfluence 14 keV 31P ions implanted into Si with atomic scale accuracy. Atom Probe Tomography is based on the highly controlled field-evaporation of individual ions from the surface of a very-sharp needle-shaped specimen. It provides a 3D reconstruction of the distribution of implanted ions, typically within a volume of 80 x 80 x 200 nm3 , which can be imaged to a spatial precision better than 1 nm and a chemical sensitivity of less than 0.01 at.%. We observe that the experimental depth profile has a FWHM of 20 nm with a depth consistent with the SRIM simulations. We review the propects for the fabrrcaiton of nanoscalse arrays with the top-down deterministic ion implantation method.atoms [2] for various quantum technologies.

Acknowledgements: Supported by the ARC Centre of Excellence for Quantum Computation and Communication Technology. We acknowledge the collaboration of the Atom Probe Research Group, Department of Materials, University of Oxford, UK.

J.T. Muhonen, J-P. Dehollain, A. Laucht, et al., Storing quantum information for 30 seconds in a nanoelectronic device, Nature Nanotechnology 9, p986-991 (2014)
J.A. van Donkelaar, C. Yang, A.D.C. Alves, et al., Single atom devices by ion implantation, Journal of Physics: Condensed Matter, 27, 154204 (2015)

Professor David Norman Jamieson

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David is a Professor of Physics at the University of Melbourne and Head of the School of Physics of the University of Melbourne. This is one of the leading Physics Schools in Australia. He completed his PhD in physics at the University of Melbourne in 1985 and then spent 4 years working at Caltech (USA) and the University of Oxford (UK) as a postdoctoral research fellow.

His research expertise in the field of ion beam physics, particularly in the use of focused ion beams for materials modification and analysis. He has developed single ion implantation techniques for the deterministic doping of semiconductor devices and for charge injection and transport studies. A key outcome to date has been the successful fabrication of a nanoscale device that has demonstrated the control and readout of single electron and nuclear spins of an engineered ion implanted phosphorus donor atom. This device is being used to test some of the key functions of a revolutionary quantum computer constructed in silicon in the Australian Research Centre of Excellence for Quantum Computation and Communication Technology where he is a program manager. His deterministic doping technique is cited in the 2011 International Technology Roadmap for Semiconductors.

He has been a finalist in the Australian Awards for University Teaching and has published over 260 papers in scientific journals and 1 book. He served as President of the Australian Institute of Physics from 2005 to 2006 and is a Fellow of the AIP and the Institute of Physics UK. He also gives numerous annual public lectures around Australia on fundamental questions in Physics. From 2010 to 2012 he convened a national working group to develop the Decadal Plan for Physics in Australia which was submitted to the Academy of Science in December 2012.

Surface-confined polymerization by Ullmann and Schiff-base coupling reactions

Giorgio Contini

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Novel nanostructured low-dimensional materials have received marked interest in the last decade since they could be employed as active media in organic electronics devices. Graphene-like two-dimensional organic materials can be grown and confined with different strategies onto suitable surfaces depositing and activating selected molecules. In this respect, the surface-confined polymerization is a very promising bottom-up approach that allows the creation of layers with desired architectures and tunable properties changing the molecules used as precursor.

In this talk I will report on some of the progresses made on surface-confined polymerization and on our studies on π-conjugated polymeric structures obtained in ultra-high vacuum (UHV) and at the solid-water interface by using Ullmann and Schiff-base coupling reactions, respectively.

The Ullmann reaction, obtained for 1,4-dibromobenzene ($C_6H_4Br_2$) on Cu(110), will be discussed by complementary spectroscopic measurements of occupied and unoccupied states (using photoelectron spectroscopy (XPS, ARUPS) and near edge X-ray absorption fine structure (NEXAFS) spectroscopy, respectively), scanning tunneling microscopy (STM) and density functional theory (DFT). These methodologies have allowed to pinpoint a signature of the polymerization reaction and have added new information on the role played by the halogen atom in the organometallic intermediate structure. Fast-

XPS measurements performed during the annealing of the surface provided real-time information about the transition. A comparison with 1,4-halobenzene molecules having different halogen atoms on the Cu(110) surface will be presented.

Schiff-base reaction, which involves amines and aldehydes as building blocks, has been explored at the solid-water interfaces. 4,4’-diaminostilbene dihydrochloride and terephtalaldehyde have been studied in solution and onto iodine-modified Au(111) in water, analyzed in situ by STM and ex situ by XPS, to obtain information on polymerization. A spectroscopic evidence of the surface-confined polymer formation as a function of the pH has been found, confirming the validity of the proposed Schiff-base method, so far studied mainly by local probe techniques. Insights into the catalytic effect of the substrate and the reaction steps will be shown.

Dr Giorgio Contini

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Giorgio Contini is Researcher and Laboratory Head at the Istituto di Struttura della Materia (ISM), National Research Council (CNR) and Acting Professor at the Physics Department, Tor Vergata University, Roma, Italy. Born in Roma (Italy) in 1963, he got a PhD in Materials for Health, Environment and Energy from University “Tor Vergata”, Roma, Italy and a MSc in Physics from University “La Sapienza”, Roma, Italy. Researcher from 1988 to date at CNR, since 2002 he is the head of a surface science laboratory (IC11-SSL, ISM). Since 1990 he is leader for the CNR unit of various scientific activity and contracts, funded by European community and Research and Education Ministry of Italy. He is the scientific coordinator of projects on different European synchrotron radiation sources and thesis supervisor~~s~~. He is member of the American Chemical Society (ACS), Italian Physical Society (SIF) and Italian Society of Synchrotron Light (SILS). Editorial Board Membership: International Journal of Nanoscience, Current Physical Chemistry. Research areas of interest are Surface Science, Organic molecules, Nanostructured Materials. Research sub-fields: self-assembled molecular structures, 2D polymerization, supramolecular assemblies, chirality, advanced spectroscopic techniques, synchrotron radiation.

The research activity has been developed in the molecular physics and chemical physics of surfaces fields. The main actual research interest is the study of organic molecules both in gas phase and adsorbed on surfaces, with particular emphasis to chiral surfaces and surface-confined polymerization by Ullmann and Schiff-base coupling reactions. The principal aim of the research is the developing of devices based on molecules to be used in electronic and as sensors. Basic studies are devoted to the determination of binding, growing mechanism, geometry and orientation of the molecules on different surfaces. Results obtained in gas-phase are correlated with those obtained on surfaces. The properties of nanostructured materials, and the control of their size, shape, composition, stability and positioning when grown on suitable substrates are studied by using traditional and advanced spectroscopic techniques by laboratory and synchrotron radiation sources: electron and photon stimulated desorption (EDS, PDS), photoelectron spectroscopy (XPS, UPS and XPD), Auger (AES), near edge X-ray absorption spectroscopy (NEXAFS, XANES), scanning tunneling microscopy (STM), low energy electron diffraction (LEED), infrared spectroscopy (IR) and circular dichroism in the angular distribution of photoelectrons (CDAD).

He is author of more than 65 scientific papers published in IF Journals, and invited speaker, scientific organizer and chair of sessions at international Conferences.

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STM Imaging of the transition from SiC to graphene

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We studied by Scanning Tunneling Microscopy the different atomic reconstructions of 3C---SiC/Si after high temperature annealing in Ultra High Vacuum, leading to the formation of Graphene. Graphene obtained from thermal decomposition of 3C---SiC/Si is more appealing in terms of cost effectiveness compared to the one obtained from bulk SiC. Additionally, thermal decomposition in ultra---high vacuum (UHV) gives origin to a contaminant free surface.

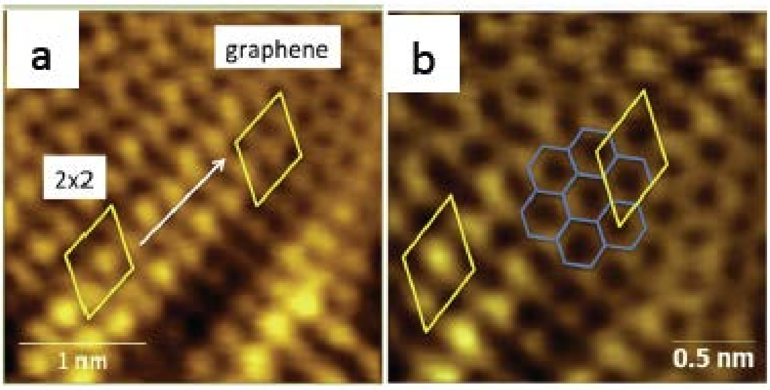

Figure 1 -- STM images of the transition from SiC to graphene: bias---0.02 V; current---80 pA. a) image of a 2x2 region where it is possible to observe the transition from the bottom left to top right. b) a zoom of the transition region

Graphene was obtained by annealing 3C SiC/Si (111) substrates in UHV for 10 mins at 1250 ˚C [1]. Atomic resolution images of the surface show the transition from a nominal R30°(√3x√3) to a R30°(3/2x√3) reconstruction of the Si terminated layer. A distortion of the surface cell is occurring in the transition regions, caused by the rearrangement of Si atoms, and leading to a 2x2 reconstruction, which gradually disappears to leave place to the graphene structure (Fig 1).

This is the first time that the SiC to graphene transition is clearly imaged by STM[2]. We present also a DFT model of the atomic reconstruction giving account of the experimental findings.

References

1. Gupta, B., M. Notarianni, N. Mishra, M. Shafiei, F. Iacopi, and N. Motta, *Evolution of epitaxial graphene layers on 3C SiC/Si (111) as a function of annealing temperature in UHV.* Carbon, 2014. **68**: p. 563---572.
2. Gupta, B., E. Placidi, C. Hogan, N. Mishra, F. Iacopi, and N. Motta, *The transition from 3C SiC(111) to graphene captured by Ultra High Vacuum Scanning Tunneling Microscopy.* Carbon, 2015. **91**: p. 378---385.

Professor Nunzio Motta

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Professor Nunzio Motta obtained his Laurea in Physics in 1981 (Università La Sapienza – Roma) and his PhD in Physics in 1986 (Scuola Normale Superiore - Pisa). He is internationally recognized in the field of material science, with over 25 years experience in growth and characterization of nanostructures, mainly acquired in Italy, where he became a leader in surface science and epitaxial growth of semiconductors. He is currently leading research at QUT in solar energy and environmental nanotechnology, developing graphene based supercapacitors, new polymer solar cells and solar powered nano-sensors. Nunzio obtained several visiting positions in various research institutions across Europe, published more than 130 papers in material science and surface physics and led many international research projects in the area of nanotechnology. He is chair of the conference NanoS-E3 since 2007.

Observation of Plasmon Resonances in Two-Dimensional MoS_2

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Research on two-dimensional (2D) transition metal dichalcogenides and especially 2D molybdenum disulfide (MoS_2) has increased rapidly in recent years [1-5]. Plasmonics of 2D MoS_2 have attracted attention due to their desirable dispersion relation, eliminating the cutoff frequency limit [6, 7]. Additionally their large tuneability, high doping (ultradoping) range, and the existence of favorable depolarization factors allow for their better control. Challenges remain regarding the generation of plasmons in intrinsic 2D MoS_2, which accommodates massive electrons (unlike graphene) and relatively low carrier concentrations (10^{12} to 10^{14} cm^{-3}) [6]. Consequently, it has been theoretically shown that intrinsic 2D MoS_2 plasmon resonances only appear at relatively low frequencies, in the far-infrared and terahertz regimes. Hence, doping is crucial to increase the carrier concentration in order to obtain plasmon resonances at commercially useful wavelengths. Additionally, the demonstration of plasmon harvested energy at such wavelengths can be potentially used for in vivo therapeutic applications and catalysis.

We have previously shown plamonc resonances in strongly intercalated 2D MoO_3 [8]. In this work, by electrochemically intercalating lithium into 2D MoS_2 nanoflakes, plasmon resonances in the visible and near UV wavelength ranges are achieved [9]. These plasmon resonances are controlled by the high doping level of the nanoflakes after the intercalation, producing two distinct resonance peak areas based on the crystal arrangements. The system is also benchmarked for biosensing using bovine serum albumin. This work provides a foundation for developing future 2D MoS_2 based biological and optical units with plasmonic functionalities.

1. Berean, K.J., et al., *2D MoS_2 PDMS Nanocomposites for NO_2 Separation.* Small, 2015: DOI: 10.1002/smll.201501129.
2. Nguyen, E.P., et al., *Investigation of two-solvent grinding-assisted liquid phase exfoliation of layered MoS_2.* Chemistry of Materials, 2015. **27**(1): p. 53-59.
3. Ou, J.Z., et al., *Ion-driven photoluminescence modulation of quasi-two-dimensional MoS_2 nanoflakes for applications in biological systems.* Nano Letters, 2014. **14**(2): p. 857-863.
4. Wang, Y., et al., *Electrochemical control of photoluminescence in two-dimensional MoS_2 nanoflakes.* ACS Nano, 2013. **7**(11): p. 10083-10093.
5. Wang, Q.H., et al., *Electronics and optoelectronics of two-dimensional transition metal dichalcogenides.* Nature Nanotechnology, 2012. **7**(11): p. 699-712.
6. Scholz, A., T. Stauber, and J. Schliemann, *Plasmons and screening in a monolayer of MoS_2.* Physical Review B - Condensed Matter and Materials Physics, 2013. **88**(3): p. 035135.
7. Naik, G.V., V.M. Shalaev, and A. Boltasseva, *Alternative plasmonic materials: Beyond gold and silver.* Advanced Materials, 2013. **25**(24): p. 3264-3294.
8. Alsaif, M.M.Y.A., et al., *Tunable plasmon resonances in two-dimensional molybdenum oxide nanoflakes.* Advanced Materials, 2014. **26**(23): p. 3931-3937.
9. Wang, Y., et al., *Plasmon resonances of highly doped two-dimensional MoS_2.* Nano Letters, 2015. **15**(2): p. 883-890.

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Kourosh Kalantar-zadeh is a Professor and Director of the Centre for Advanced Electronics and Sensors (CADES) at RMIT University, Australia. He received his B.Sc. (1993) and M.Sc. (1997) degrees at Sharif University of Technology, Iran, and Tehran University, Iran, respectively, and his Ph.D. at RMIT University, Australia (2002). His research interests include chemical and biochemical sensors, nanotechnology, microsystems, materials science, electronics, microfluidics and gastroenterology. Kourosh is the author of over 320 peer reviewed scientific papers and books.

Molecular Self-assembly on Graphene vs Graphite

Dr Josh Lipton-Duffin, Senior Research Officer

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Graphene has excellent strength, flexibility, and charge mobility, yet lacks certain desirable properties that would render it more useful for applications. In particular, graphene has no band gap, and as such cannot be used as the active material in semiconductor devices. Much effort has been devoted to engineering a solution to this problem, either by creating new, graphene-like materials from bottom-up, or by altering or modifying graphene from the top down. In the context of this latter approach, it has been theorised that a self-assembled coating of molecules on a single-layer graphene (SLG) surface may modify its electronics in a way that opens a band gap, thereby converting the semimetal into a semiconductor. As the behaviour of small molecules on a surface depends critically on both molecule-substrate and molecule-molecule interactions, we have explored the feasibility of using well-known assemblies on highly-oriented pyrolitic graphite (HOPG) as a proxy for assembly on SLG. We find that identical self-assembled monolayers persist on cu-supported SLG in exactly the same way as on HOPG, and that the self-assembled layer is able to adapt to the rumpling of the layer. The findings are demonstrated through use of scanning tunnelling microscopy (STM) at the solution-solid interface, and are supported by first-principles calculations using density functional theory (DFT).

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Dr Lipton Duffin obtained his PhD in Physics at Queen's University Kingston, Ontario in 2006. He has strong skills in experimental techniques of surface science and associated instrumentation, with primary competencies in photoelectron spectroscopies (x-ray photoelectron and angle-resolved inverse photoelectron) and scanning tunneling microscopy (STM). He is proficient at epitaxial overlayer growth on metals and semiconductors, and has an extensive experience in LEED/Auger, X-PEEM and XRD both in laboratory and synchrotron environments. He published more than 45 papers in high impact factor International reviews (Small, ACS Nano, review of scientific instruments), with 457 citations and an h-index of 11.

At QUT since 2015 he is responsible of the surface science labs at the Central Analytical research Facility, conducting research in 2D materials and molecular self-assembly on surfaces.

Molecular trapping with a monolayer covalent organic framework

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Covalent organic frameworks (COFs) are a recently-discovered class of porous crystalline materials.[1] COFs have high specific surface areas due to their nanoscale pores, and together with their high thermal stability and the fact that they can be synthesized from a range of basic building blocks, they are appealing candidates for applications ranging from gas storage to photovoltaics.[2]

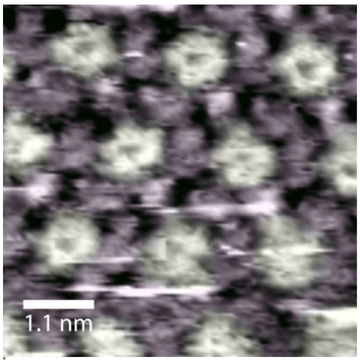

Figure 8: Scanning tunneling microscopy image showing guest molecules (pale yellow) in a COF host lattice (purple).

COFs are commonly synthesized as three-dimensional (bulk) materials. However, surface-confined monolayer COFs present an advantage for some applications, since they can be easily integrated into standard device geometries. Here, I will discuss recent work in which we have used two-dimensional surface-confined COFs to trap fullerene molecules. This process effectively defines a host/guest structure from the COF lattice and fullerenes. The host/guest structure can be synthesized at the solution/solid interface and is also stable after allowing the solvent to dry. I will discuss our characterization of the structure and energetics of this system, as well as discussing the possible applicability of this approach to applications in sensing .

[1]. A. P. Cote, A. I. Benin, N. W. Ockwig, M. O'Keeffe, A. J. Matzger and O. M. Yaghi, Science, 2005, 310, 1166-1170.

[2]. S.-Y. Ding and W. Wang, Chemical Society Reviews, 2013, 42, 548-568.

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Jennifer MacLeod holds a PhD in Physics from Queen's University in Kingston, Canada. Since receiving her PhD in 2006, she has worked as a Postdoctoral Fellow and Research Associate at the Centre Énergie, Matériaux et Télécommunications of the Institut national de la recherche scientifique (INRS-EMT, Varennes, Canada) and as a Natural Science and Research Council of Canada (NSERC) Postdoctoral Fellow at the Universita degli Studi di Trieste (Trieste, Italy). Dr. MacLeod specializes in condensed matter physics at the nanoscale, with particular interests in surface science and surface chemistry. Her primary research focus is on elucidating and controlling surface-confined molecular assemblies and reactions using a combination of high-resolution microscopy, spectroscopy and quantum chemistry calculations. She is also interested in instrument development, with the aim of developing new tools for nanoscale characterization and synthesis of materials. In February 2015, Dr. MacLeod joined the QUT School of Chemistry, Physics and Mechanical Engineering as a Senior Research Fellow in Surface Science.

Graphene and other 2d crystals for energy devices

Vittorio Pellegrini

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NEST CNR-NANO and Scuola Normale Superiore, Pisa (Italy)

Energy conversion and storage are two of the grand challenges that our society is facing. New materials and processes [1] can improve the performance of existing devices or enable new ones that are also environmentally benign. In this talk we will start by reviewing recent progresses on the large-scale production of graphene, two-dimensional crystals and related composites for industrial applications [2]. We will then focus on energy conversion and storage [3] and, particularly, on our recent developments of graphene-based ink battery that displays an estimated energy density of about 200 $\mathrm{Whkg^{-1}}$ and a stable operation for over 80 charge-discharge cycles [4]. These properties are linked to the graphene nanoflake anode displaying crystalline order and high uptake of lithium at the edges. We also discuss the role of the graphene nanoflake morphology on the mechanism of lithium uptake highlighting the impact of the number of graphene layers and nanoflake lateral sizes on irreversible/reversible capacities [5]. Our approach, compatible with any printing technologies, is cheap and scalable and opens up new opportunities for the development of high-capacity Li-ion batteries.

1. F. Bonaccorso, et al., Production and processing of graphene and 2d crystals. *Materials Today*, **15**, 564 (2012).
2. P. Cataldi, et al., Foldable Conductive Cellulose Fiber Networks Modified by Graphene Nanoplatelet-Bio-based Composites *Adv. Electronic Materials*
3. F. Bonaccorso, et al., Graphene, 2d crystal and hybrid structures for energy conversion and storage. *Science* **347**, 1246501 (2015).
4. J. Hassoun, et al. An advanced lithium-ion battery based on a graphene anode and a lithium iron phosphate cathode. *Nano Lett.* **14**, 4901-4906 (2014).
5. H. Sun et al. *in preparation*

Professor Vittorio Pellegrini

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NEST CNR-NANO and Scuola Normale Superiore, Pisa (Italy)

Vittorio Pellegrini's research interests focus on the physics and application of low-dimensional semiconductor systems and graphene. During his research carrier he discovered several fundamental collective phenomena and quantum phase transitions in quantum Hall nano-systems by means of inelastic light scattering, magneto-optics and magneto-transport. He has also applied the most advanced optical spectroscopy techniques to investigate several biomolecular processes in living cells. Recently he developed optical methods for the control of the electronic properties of few correlated electrons in single quantum dots. Additionally he and his group have realized an artificial version of graphene by nanofabricating a two-dimensional honeycomb lattice on the surface of a semiconductor material. The most recent activities focus on graphene and other two-dimensional (2D) crystals. In particular he is exploring the use of graphene and other 2D materials for energy applications. The most technological oriented activities deal with the large-scale production of 2D crystals inks and graphene composites for industrial applications. Currently he is the director of the IIT Graphene Labs, leader of the energy storage workpackage of the Graphene Flagship and scientific secretary of the strategic advisory council of the Graphene Flagship. He has published more than 150 papers in peer-reviewed journals. He has been visiting professor at Columbia University (USA) and University of Lancaster (UK).

Compound semiconductor nanowire solar cells

Lan Fu, Qian Gao, Lan Fu, Li Li, Kaushal Vora, Ziyuan Li, Fan Wang, Zhe Li, Yesaya Wenas, Sudha Mokkapati, Fouad Karouta, Hark Hoe Tan, and Chennupati Jagadish

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Semiconductor nanowires (NWs) have received increasing attention in recent years for solar cell applications, due to 1) their intrinsic antireflection property for enhancing light absorption; 2) their small footprints efficiently relaxing the lattice-mismatched strain and thus enabling the construction of multi-junction solar cells with optimal band gap combinations and/or the growth on different substrate materials such as silicon; and 3) significant cost reduction due to much less material usage. With highly suitable bandgap, superior carrier mobility and well-developed synthesis techniques, axial p-i-n junction InP nanowire array solar cells have been reported with significantly improved performances (up to 13.8%) recently [1]. In order to achieve efficient light absorption and carrier collection in the NW solar cells (NWSCs), the critical optimisation involves not only the array geometry design in terms of NW diameter, height and spacing, but also a much more complicated junction design in terms of the length, position and doping concentration of different structral segments [2]. Furthermore, due to the nanoscale device size and complex growth dynamics regarding dopant incorporation, diffusion, and growth rate variation simultaneously occurring during the NWSC growth, it is essential to characterise the pn junction of NWSC in order to understand the solar

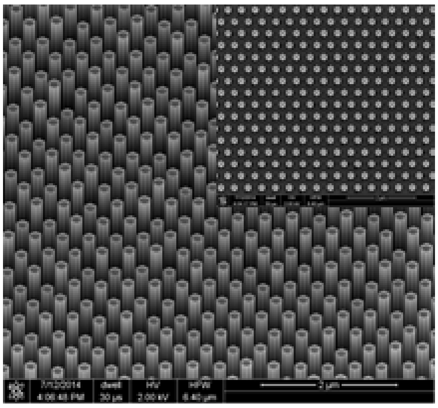

Figure 9 Scanning electron microscopy (SEM) image of an InP NW array solar cell grown by MOVPE technique.

cell device behavior. In this work we will present our research at the Australian National University on design (coupled optical and electrical numerical simulation), growth (selective area metal-organic chemical vapour deposition (SA-MOCVD)), fabrication and characterisation of InP nanowire solar cells. In particular, we will demonstrate the importance of using electron beam induced current (EBIC) technique to directly characterise/visualise the pn junctions in various NWSC designs to achieve improved device performance.

1. J. Wallentin et al., InP nanowire array solar cells achieving 13.8% efficiency by exceeding the ray optics limit. Science, 2013, **339**: p.1057.
2. Z. Li et al., Influence of Electrical Design on Core–Shell GaAs Nanowire Array Solar Cells. IEEE Journal of Photovoltaics, 2015, **5** (3): p. 854.

Sustainable natural polymers for energy storage devices

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A series of novel green electrode manufacturing technologies are developed by adopting and functionalizing sustainable natural polymers in order to improve the conductivity and mechanical strength for high performance and long life lithium ion batteries [1, 2]. As an example, the naturally occurring binder sodium alginate (SA) is functionalized with 3,4-propylenedioxythiophene-2,5-dicarboxylic acid (ProDOT) via a one-step esterification reaction in a cyclohexane/dodecyl benzene sulfonic acid (DBSA)/water micro-emulsion system, resulting in a multi-functional polymer binder i.e., SA-PProDOT. With the synergetic effects of the functional groups (e.g., carboxyl, hydroxyl and ester groups), the resultant SA-PProDOT polymer not only maintains the outstanding binding capabilities of sodium alginate, but it also enhances the mechanical integrity and lithium ion diffusion coefficient in the $LiFePO_4$ (LFP) electrode during the operation of the batteries. Due to the conjugated network of the PProDOT and the lithium doping under the battery environment, the SA-PProDOT becomes conductive and matches the conductivity needed for LiFePO4 LIBs. Without the need of conductive additives such as carbon black, the resultant batteries have achieved the theoretical specific capacity of LiFePO4 cathode (ca. 170 mAh/g) at C/10 and ca. 120 mAh/g at 1C for more than 400 cycles.in a multi-functional polymer binder i.e., SA-PProDOT. With the synergetic effects of the functional groups (e.g., carboxyl, hydroxyl and ester groups), the resultant SA-PProDOT polymer not only maintains the outstanding binding capabilities of sodium alginate, but it also enhances the mechanical integrity and lithium ion diffusion coefficient in the

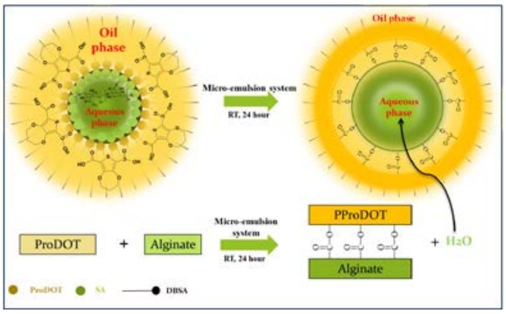

Figure 10, Functionalization of alginate

$LiFePO_4$ (LFP) electrode during the operation of the batteries. Due to the conjugated network of the PProDOT and the lithium doping under the battery environment, the SA-PProDOT becomes conductive and matches the conductivity needed for LiFePO4 LIBs. Without the need of conductive additives such as carbon black, the resultant batteries have achieved the theoretical specific capacity of LiFePO4 cathode (ca. 170 mAh/g) at C/10 and ca. 120 mAh/g at 1C for more than 400 cycles.

Reference

1. Multifunctional SA-PProDOT Binder for Lithium Ion Batteries, ***Nano Lett.*** 2015, , DOI: 10.1021/acs.nanolett.5b00795
1. Dual-functional gum arabic binder for silicon anodes in lithium ion batteries, ***Nano Energy,*** 2015***,*** 12, 178–185

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A/Prof. Shanqing Zhang obtained his PhD degree in electrochemistry in 2001 at Griffith University, Australia. Since then, he has been working on synthesis, modification, characterisation of nanostructured materials for sensing, energy conversion and energy storage devices. As a core inventor, Dr. Zhang has developed a series of patented and commercialized photoelectrochemical sensors for environmental monitoring based on the functional nanomaterials. He was awarded Australia Research Council Future Fellow in photoelectrocatalysis for 2009-2013. Currently, Dr. Zhang is leading his group conducting research on energy conversion and storage.

Nanotechnology: new paradigms for nanomedicine

Fabio Beltram

Laboratorio NEST

Scuola Normale Superiore, Pisa, Italy

Our increased ability to tailor molecule and, more in general, nanosystem properties can be exploited to design and produce *intelligent* tags that *analyze* and *react to* the cellular environment. Today multifunctional nanosystems can be produced that provide a signal or a function dependent on the value of a specific biochemical parameter. Importantly these nanosystems can target specific subcellular domains and have the ability to be used also in the case of live organisms.

Recent results will be discussed that highlight the impact of nanobiotechnology in this context with a particular emphasis given to methods suitable for *in vivo* studies that can be transferred to biomedical world (see Fig 1). These studies are producing the building blocks of nanomedicine a *new* medicine with strong emphasis on prevention that may make the concept of *magic bullet* a reality.

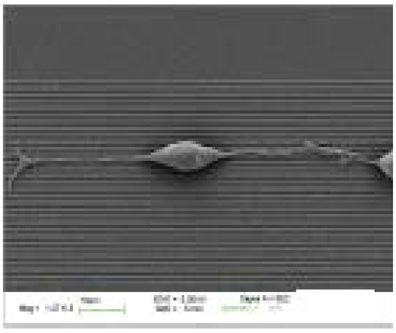
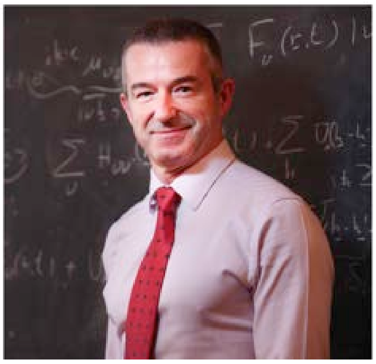


Figure 2. Example of nanopatten --- driven cell differentiation.

Additionally I shall show that these nanotools can be integrated in lab---on---a--- chip architectures to provide fast, automated diagnostic functions and tailorable environments for guided cell growth and differentiation (see Fig. 2). In this context a novel on --- chip pumping protocol based on surface acoustic waves will be shown also within complex fluidic networks. This approach eliminates the need for external pumps or circuitry and opens the way to fully stand--- alone miniaturized fluidic chips.



Professor Fabio Beltram

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Fabio Beltram obtained Doctor Degrees in Physics and in Electronic Engineering. He carried out research activity at Bell Laboratories (Murray Hill, NJ, USA) until 1992 when he moved to the Scuola Normale Superiore (Pisa, Italy) where he is now Professor of Physics of Matter and Director of the Nanoscience Laboratory (Laboratorio NEST).

At present he is Director of Scuola Normale Superiore. Fabio Beltram is Fellow of the American Physical Society and Senior Member of IEEE.

Fabio Beltram and his group carry our research work in the field of nanoscience and nanotechnology with a rather broad spectrum of topics. His results appeared in about four hundred publications in international journals and patents. He has always worked on the physics and applications of semiconductor and hybrid superconductor-semiconductor nanostructures. Increasingly in the last years Fabio Beltram has carried out research activity in the field of molecular biophysics in order to apply his expertise in nanotechnology and in the engineering of nanostructures to significant issues in nanobiotechnology and biomedicine.

Biomimetic mineralization of metal-organic frameworks from biomacromolecules

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Many natural living organisms fabricate rigid exoskeletons for the protection of soft tissues[1]. This synthetic mechanism, termed biomineralization, involves fine control of crystal morphology and chemical composition of the biominerals[2]. This natural process has inspired 'biomimetic' strategies for the preparation of new materials for drug delivery, biomedical implants, and biochemical separations. Here, we present the first example of biomimetic mineralization of metal-organic frameworks (MOFs)[3]. Such a biologically inspired self-assembly process leads to the formation of a highly porous MOF shell around biomacromolecules (Figure 1) including proteins, enzymes, and DNA, with distinctive crystal morphology.

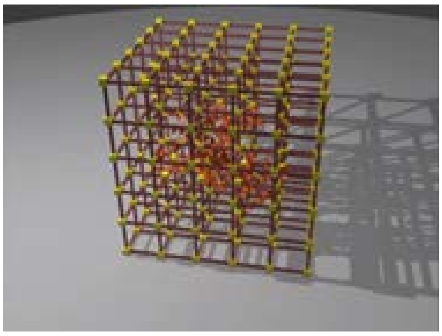

Figure 11. Schematic illustration of biomimetic mineralization of metal-organic frameworks (MOFs).

As a result, the porous MOF shell allows for the selective transport of small molecules, regulating the interaction between active biomacromolecule (e.g. enzymes) and the external environment. Remarkably, the stability of the biomacromolecules is considerably enhanced. Moreover, the biomimetically mineralized MOF coatings can be engineered responsive to biological triggers, which enable the release of the protected cargo on demand. This discovery proposes MOFs as an ideal class of candidate materials for a range of biotechnological applications, such as industrial biocatalysis, drug delivery, and biomedical lab-on-a-chip device fabrication[3,4].

References

[1] Estroff, L. A. *Chem. Rev.* 2008, 108 (11), 4329.

[2] Meldrum, F. C.; Cölfen, H. *Chem. Rev.* 2008, 108 (11), 4332.

[3] Liang, K.; Ricco, R.; Doherty, C. M.; Styles, M. J.; Bell, S.; Kirby, N.; Mudie, S.; Haylock, D.; Hill, A. J.; Doonan, C. J.; Falcaro, P. *Nat. Commun.* 2015, 6, 7240.

[4] Falcaro, P.; Ricco,R.; Doherty, C. M.; Liang, K.; Hill, A. J.; Styles M. J. *Chem. Soc. Rev.* 2014, 43, 5513.

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Kang Liang received his PD degree in Chemical Engineering from the University of Melbourne, developing nanoengineered particles for biomedical applications. He is currently a Postdoctoral Fellow at CSIRO, where he is utilizing his expertise in developing functional porous materials for biotechnology.

Bio-inspiration: a new path to reach multifunctional nanomaterials

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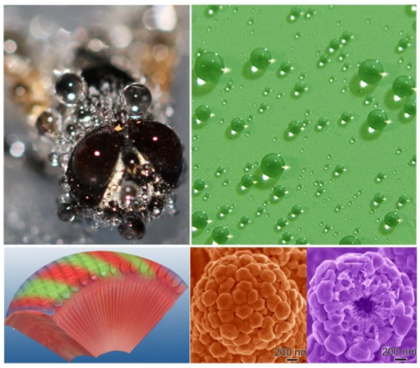
Learning from nature takes ideas from natural species and develops novel functional materials based on these concepts, *e.g.*, bio-inorganic materials (biomineralization), bio-inspired multiscale structured materials (chiral morphologies), bio-nanomaterials (bio-nanoparticles), hybrid organic/inorganic implant materials (bonelike composites), and smart biomaterials. Many of these smart materials have surfaces that dynamically alter their physicochemical properties in response to changes in their environmental conditions and to triggered control of interfacial properties.

In our research, by mimicking the well-ordered multiscale structures of natural interfaces or surfaces, many inorganic nanomaterials with bio-inspired structures and functions have been designed. For example, to develop effective anti-fogging nanomaterials that can provide protection for such surfaces, even when exposed in extreme environments, we designed fly-eye inspired superhydrophobic anti-fogging nanomaterials that have a low adherence force to water droplets and thus resist fogging-induced ice build-up. The development of the fish-scale bio-inspired inorganic nanostructures, which have similar multiscale structures and multiple-functions to that of the natural targets, greatly extends the applications of bio-inspired materials to fields from micromechanical devices to heavy-duty machines as protective coatings against mechanical damage and



chemical corrosion, as optical elements in optical devices and photovoltaic energies, and as low-drag or low-friction surfaces in gaseous, liquid, and solid media, etc. Therefore, we believe that the design of bio-inspired nanostructures could provide a new approach for develop novel multifunctional nanomaterials in the future.

References:

1. Z. Q. Sun, T. Liao, K. Liu, L. Jiang, J. H. Kim, S. X. Dou, *Small*, **10**, 3001-3006 (2014)
2. Z. Q. Sun, T. Liao, W. Li, K. Liu, L. Jiang, S. W. Kim, J. H. Kim, S. X. Dou, *NPG Asia Mater.*, in press (2015)

Transparent conducting electrodes for organic electronic devices

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Organic solar cells (OSCs) and organic light emitting diodes (OLEDs) require a transparent conducting electrode for in-coupling and out-coupling of light, respectively. A transparent conducting electrode should have high transmittance in the visible region and a very low sheet resistance (high conductivity).

Since the inception of these devices [1, 2], the most commonly used transparent conducting electrode is indium tin oxide (ITO). Commercial ITO electrodes are widely used for organic electronic devices. This is because ITO has an excellent combination of high transmittance (~ 90%) and a very low sheet resistance (~15 ohms/sq.). In addition, ITO films are highly reproducible and give consistent results. However, there are certain disadvantages of ITO including inflexibility, increasing cost of indium due to increasing demands of ITO from organic electronic industry, instability of devices etc. Therefore, finding alternatives to ITO is a major area of research. Some of the alternatives are doped metal oxides, organic polymers, metal grids, carbon nanotubes and graphene [3, 4]. In this talk, I will review a few recent electrode materials and their applications in organic electronic devices (OSCs and OLEDs).

1. Tang, C.W., *2-Layer organic photovoltaic cell*. Applied Physics Letters, 1986. 48: p. 183-185.
2. Tang, C. W. & VanSlyke, S. A., *Organic electroluminescent diodes*. Applied Physics Letters, 1987. 51: p. 913–915.
3. Liao, KS., et al., *Designs and architectures for the next generation of*

organic solar cells. Energies, 2010. 3(6): p. 1212-1250.

4. Cao, W., *Transparent electrodes for organic optoelectronic devices: a review.*

   Journal of Photonics for Energy, 2014. 4(1): p. 040990.

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Soniya D. Yambem is a Vice-Chancellor's research fellow at QUT. Soniya is a device physicist with extensive experience in fabricating flexible electronic devices. Before joining QUT she worked on CSIRO's flagship cluster project in flexible electronics at the University of Queensland. In her current role as a VC Fellow at QUT, Soniya is working with a team of highly acclaimed scientists from diverse fields such as tissue engineering, 3-D printing and organic chemistry to pursue her passion in developing the next generation of wearable electronic technology for medical applications.

High Performance Printable Donor-Acceptor Based Organic Semiconductors for Novel Organic Electronic Devices

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Organic semiconductors are the focus of intense academic and industrial research because they are important functional materials for low cost printable electronics, particularly OTFTs and OPVs. These materials are emerging as an interesting category for these applications due to their relatively adequate HOMO-LUMO energies, tunable light absorption and attractive charge transport properties [1].

In this presentation, the design, synthesis, optoelectronic properties, solid state interactions and device performance of newly developed organic semiconductors will be discussed. Some novel materials could achieve high hole carrier mobility close to 1 to 4.2 cm^2/Vs in p-channel OTFTs with low operating voltage (< 10 V) and small channel length (4 microns)[2-5]. Our rationally designed materials also exhibited highest hole (0.75 cm^2/Vs) and electron (1.45 cm^2/Vs) mobility in ambipolar OTFTs. This ambipolar polymer also used successfully for logic circuits and memory devices [7-9]. OPV devices made up of these materials exhibited 5% power conversion efficiency (PCE) in bulk heterojunction (BHJ) solar cells. Our efforts toward development of non-fullerene acceptors will be also discussed.

[1] Y. Li, P. Sonar, L. Murphy, W. Hong, Energy and Envi. Sci. 2013, 6, 1684

[2] Y. Li, S. P. Singh, P. Sonar, Adv. Mater., 2010, 22, 4862

[3]P. Sonar, S. P. Singh, Y. Li, Zi-En Ooi, Tae-Jun Ha, Ivy Wong, M. S. Soh and A. Dodabalapur, Energ. Environ. Sci. 2011, 22, 5409

[4] Y. Li, P. Sonar, S. P. Singh, M. S. Soh, M. van Meurs, J. Tan, J. Am. Chem. Soc., 2011, 133, 2198

[5] Y. Li, P. Sonar, S. P. Singh, W. Zeng, M. S. Soh, J. Mat. Chem., 2011, 21, 10829

[6] P. Sonar, S. P. Singh, Y. Li, M. S. Soh, A. Dodabalapur, Adv. Mater., 2010, 22, 5409

[7] P. Sonar, T. R. B. Foong, S. P. Singh, Y. Li, A. Dodabalapur, Chem. Commun. 2012, 48, 8383

[8] D. Gentili, P. Sonar, F. Liscio, T. Cramer, L. Ferlauto, F. Leonardi, S. Milita, A. Dodabalapur, M. Cavallini, Nano Letters, 2013, 13, 3643

[9] Y. Zhou, S. T. Han, P. Sonar, V. A. L. Roy, Scientific Report, 2013,3, 2319.

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Dr. Sonar performed his doctoral work under the supervision of Professor Müllen at Max- Planck Institute of Polymer Research, Mainz, Germany and was awarded his *PhD* in 2004 from Johannes-Gutenberg University in Mainz. Dr. Sonar moved to Swiss Federal Institute of Technology (ETH), Zurich, Switzerland for doing his postdoctoral research as a postdoctoral scientist with Professor Schlüter from 2004 till 2006. Since August 2006, he has been working in a Visiting Investigator Program (VIP) group as a Research Scientist at Institute of Materials Research and Engineering (IMRE), Agency of Science, Technology and Research (A*STAR). Dr. Sonar received prestigious Future Fellowship (2013) from the Australian Research Council and was appointed as Associate Professor at Queensland University of Technology (QUT), Brisbane, Australia SINCE July 2014.

Dr. Sonar is interested in design and synthesis of novel π-functional materials (small molecules, oligomers, dendrimers, and polymers) for printed electronics, (OFETs, OLEDs, OPVs, OLETs, OPDs, and Sensors) bioelectronics and supramoleculecular electronic applications. Dr. Sonar delivered more than 25 invited and contributed talks at various international conferences and institutes. He has authored or co-authored 82 peer-reviewed research papers in international journals (H-index-24 according to Google Scholar) and filed 11 patents and patent application in regional and international level. Recently his two patents licensed to the multinational company.

Engineering of materials for the next generation data storage memories

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Abstract: The next-generation electronic systems are expected to be light, flexible and portable for applications in large area displays, integrated circuits (ICs), light emitting diodes (LEDs), radio frequency identification (RFID) tags, solar cells and so on. Memory is an essential part of advanced electronic systems for data processing, storage and communication. Among many types of memories such as ferroelectric, electret, resistive and floating gate [1 & 2] memories, floating gate flash memory devices have gained a great deal of attention due to the simple device structure, non-destructive read-out and controlled charge trap capacity [3-5]. In this presentation, solution processed or printed materials for flash memories on plastic substrates for data storage will be discussed.

1. Su-Ting Han, Ye Zhou, and V. A. L. Roy, "Towards the development of flexible non-volatile memories", Adv. Mater., 25 (38), 5425-5449, 2013.
2. S. T. Han, Y. Zhou, C. Wang, L. He, W. J. Zhang, and V. A. L. Roy*, "Layer-by-Layer Assembled Reduced Graphene Oxide-Gold Nanoparticle Hybrid Double Floating Gate Structure for Low Voltage Flexible Flash Memories", Adv. Mater., 25 (6), 872-877, 2012
3. Ye Zhou, Su-Ting Han, Xian Chen, Feng Wang, Yong-Bing Tang and V. A. L. Roy*, "An upconverted photonic nonvolatile memory", Nature Communications, 5, 4720, 2014.
4. S. T. Han, Y. Zhou, Z. X. Xu, L. B. Huang, X. B. Yang and V. A. L. Roy*,

"Microcontact printing of ultrahigh density gold nanoparticle monolayer for flexible flash memories", Adv. Mater., 24 (26), 3556-3561, 2012

5. S. T. Han, Y. Zhou, Z. X. Xu, and V. A. L. Roy*, "Controlled ambipolar charge transport through a self-assembled gold nanoparticle monolayer", Adv. Mater., 24 (9), 1247-1251, 2012.

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Roy completed his PhD in 2004 on light emitting materials, mainly on ESR (Electron Spin Resonance) analysis of organic materials with Dr. R. B. Pode (Nagpur University), Dr. Baldacchini (ENEA, Rome) and Dr. T. K. Gundurao (IIT, Bombay). For his post-doctoral studies (with Dr. Michele Muccini at ISMN, CNR di Bologna, Italy), he focused on the growth of various organic molecules for light emitting transistors (LET) and opto-electronic characterization of LETs. In 2004, he joined the Department of Chemistry at The University of Hong Kong and he focused on various molecular materials (with Prof. Chi-Ming Che) for electronic device applications. Currently he is an Associate Professor at the Physics and Materials Science, City University of Hong Kong. He is leading a group of Physicists, Chemists and Engineers for the fabrication of functional self-assembly materials to devices and integration of such devices for printed electronics and energy harvesting devices. Over his career, he published over 100 papers in peer reviewed journals such as Nature Communications, Advanced Materials, Angew Wandte Chemie, ACS Nano, Nanoscale, Scientific Reports, Journal of Materials Chemistry, Applied Physics Letters, Chemical Communications, etc.

Magnetic Framework Composites for the uptake of Heavy Metals from water

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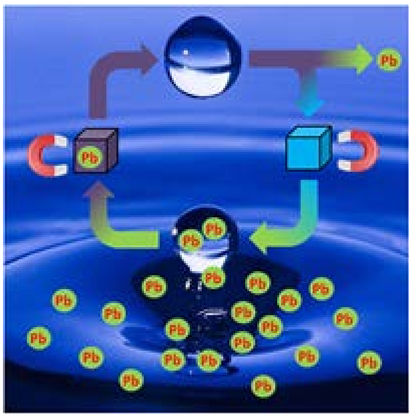
Metal Organic Frameworks (MOFs) are an emerging class of highly porous materials made of inorganic ions or clusters coordinated to organic ligands, with large surface area, tunable chemical composition, reasonable chemical and thermal stability, variable pore size distribution, and possibility of miniaturization at nanometer length scale.[1]

They can also be grown from various particles (metallic, ceramic, and polymeric particles) to produce novel composites with inherent functionality and properties for diverse potential applications. Examples have been reported with magnetic nanoparticles, having potential use in drug delivery, catalysis, sensing, as well as sequestration of several guest molecule species.[2]



Concept of lead capture and recovery from water performed by MFCs

In the last case, these magnetic composite materials can be applied to pollutant sequestration, thanks to their adsorption capabilities and their magnetic properties, permitting localization and recovery thanks to an external magnetic field. Thus, magnetic framework composites (MFCs) act as smart materials that can detect and collect environmentally and health threatening species, like polycyclic aromatic hydrocarbons (PAHs)[3] or inorganic ions.[4]

In this communication I will present the work made by our group for the synthesis, characterization of a water resistant magnetic framework composite made with an aluminium based MOF and iron oxide magnetic nanoparticles. The remarkable sequestration of Lead(II) from water will be illustrated as well.[5] In particular, the nanoporous composite reached one of the highest values obtained for this category of materials (up to ca. 500 mg g^{-1} of Pb), thus offering a novel and more effective material to harvest heavy metals from contaminated water.

[1] P. Falcaro, R. Ricco, C. M. Doherty, K. Liang, A. J. Hill, M. J. Styles, *Chem. Soc. Rev.* **2014**, *43*, 5513.

[2] R. Ricco, L. Malfatti, M. Takahashi, A. J. Hill, P. Falcaro, *J. Mater. Chem. A* **2013**, *1*, 13033.

[3] C. M. Doherty, E. Knystautas, D. Buso, L. Villanova, K. Konstas, A. J. Hill, M. Takahashi, P. Falcaro, *J. Mater. Chem.* **2012**, *22*, 11470.

[4] P. Falcaro, F. Normandin, M. Takahashi, P. Scopece, H. Amenitsch, S. Costacurta, C. M. Doherty, J. S. Laird, M. D. H. Lay, F. Lisi, A. J. Hill, D. Buso, *Adv. Mater.* **2011**, *23*, 3901.

[5] R. Ricco, K. Konstas, R. Babarao, M. J. Styles, K. Suzuki, P. Scopece, P. Falcaro, *J. Mater. Chem. A*, **2015**, (submitted).

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Raffaele Ricco completed his doctorate in molecular sciences in 2007, working on the synthesis and functionalization of carbon nanoscrolls at the University of Padua, Italy, in the group of prof. Michele Maggini. After working in the field of nanotechnology, using dye doped silica nanoparticles for DNA labeling in CIVEN/Veneto Nanotech (Venice, Italy) as researcher, in 2012 he started working in the Material Science and Engineering Division (now Manufacturing Flagship) at CSIRO Melbourne as postodoctoral fellow and later as research scientist, in the group of dr. Paolo Falcaro. His current research regards the synthesis and optimization of Metal Organic Frameworks composites with magnetic nanoparticles for environmental applications, such as heavy metal sequestration and pollution control.

Semiconductor Nanowires for Optoelectronics Applications

Professor Chennupati Jagadish, FAA, FTSE

Semiconductors have played an important role in the development of information and communications technology, solar cells, solid state lighting. Nanowires are considered as building blocks for the next generation electronics and optoelectronics. In this talk, I will introduce the importance of nanowires and their potential applications and discuss about how these nanowires can be synthesized and how the shape, size and composition of the nanowires influence their structural and optical properties. I will present results on axial and radial heterostructures and how one can engineer the optical properties to obtain high performance optoelectronic devices such as lasers, THz detectors, solar cells. Future prospects of the semiconductor nanowires will be discussed.

Professor Chennupati Jagadish, FAA, FTSE

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Professor Jagadish is an Australian Laureate Fellow, Distinguished Professor and Head of Semiconductor Optoelectronics and Nanotechnology Group in the Research School of Physics and Engineering, Australian National University. He is also serving as *Vice-President and Secretary Physical Science of the Australian Academy of Science.* Prof. Jagadish is an Editor/Associate editor of 6 Journals, 3 book series and serves on editorial boards of 17 other journals. He has published more than 820 research papers (550 journal papers), holds 5 US patents, co-authored a book, co-edited 5 books and edited 12 conference proceedings and 15 special issues of Journals. He won the 2000 IEEE Millennium Medal and received Distinguished Lecturer awards from IEEE NTC, IEEE LEOS and IEEE EDS. He is a Fellow of the Australian Academy of Science, Australian Academy of Technological Sciences and Engineering, IEEE, APS, MRS, OSA, AVS, ECS, SPIE, AAAS, IoP (UK), IET (UK), IoN (UK) and the AIP. He received Peter Baume Award from the ANU in 2006, the Quantum Device Award from ISCS in 2010, IEEE Photonics Society Distinguished Service Award in 2010, IEEE Nanotechnology Council Distinguished Service Award in 2011 and Electronics and Photonics Division Award of the Electrochemical Society in 2012, 2013 Walter Boas Medal from Australian Institute of Physics, 2015 IEEE Pioneer Award in Nanotechnology and 2015 IEEE Photonics Society Engineering Achievement Award.

Individual oxide nanowires for nano-optoelectronics

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The range of physical and chemical properties of oxide materials is overwhelming. Some of the most interesting magnetic, optical, and electronic properties are within this class of materials. Not surprisingly, oxides are at the heart of many established and emerging technologies, and, in many instances, their surfaces or their interfaces with other materials are key to device functioning. Recent achievements at SENSOR Lab will be reviewed in:

- Photoluminescence and Raman properties of individual ZnO nanowires
- Electroluminescen of ZnO NWs on p-GaN
- Plasmonic sensors.

Acknowledgments

“WIROX” Oxide Nanostructures for Wireless Chemical Sensing, PEOPLE MARIE CURIE ACTIONS, International Research Staff Exchange Scheme, Call: FP7-PEOPLE-2011-IRSES

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University of Brescia & CNR-INO – Brescia - Italy

Guido Faglia was born in 1965 and got in 1991 M.S. degree cum laude from the Polytechnic of Milan in electronics. In 1993 he was appointed Assistant Professor at the Gas Sensor Lab by the University of Brescia. In 1996 got the PhD on semiconductor gas sensors. Since 2000 he is Associate Professor in Experimental Physics at University of Brescia. In 2013 he got Italian Full Professorship habilitation as excellent in Condensed Matter Physics 02/B1 (see Annex I) . He is involved in the study of preparation of metal oxide semiconductors MOX as thin films and quasi monodimensional nanostructures for gas sensing, energy (solar cells, thermoelectrics), opto-electronic applications (LEDs) and nanomedicine. He has been involved in European Commission Projects since 1992 (Project ESPRIT No. 6374) in basic and applied physics research on semiconductors and their application in an interdisciplinary field as biochemical sensing. He has a relevant working experience with many international institutions like EC, NATO, European Space Agency ESA, INTAS. He is coordinating (2012-2015) the project WIROX in the frame of FP7-PEOPLE-2011-IRSES.

During his career Guido Faglia has published 171 articles on International Journals with referee (http://www.researcherid.com/rid/E-6991-2010). His Hirsch factor is 40 (Jul 2015); He is referee of many international journals among which Advanced Materials, Angewandte Chemie, Advanced Functional Materials and Sensors and Actuators B.

Shining Synchrotron Light on Nanoscale Electronics

Michael James,[1] Eliot Gann,[1,2] Lar Thomsen,[1] Anton Tadich[1] and Chris McNeill[2]

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Surface, interfacial and molecular interactions are ubiquitous in modern nanoscale electronics. Synchrotron X-ray based techniques are extremely well suited to the study of these systems, being highly collimated, polarized, elemental specific and surface sensitive. Of the 10 operational beamlines available at the Australian Synchrotron, two have found substantial utility in the study of nanoscale electronics: The SAXS/WAXS beamline has become a major tool for the study of the nanoscale morphology of thin-film organic semiconductors; while Soft X-ray spectroscopy beamline (SXR) is highly effective at correlating electronic function with surface composition, molecular coverage and orientation. In a number of instances it is the combined use of (Glancing Incidence)-WAXS and (Soft) Near Edge X-ray Absorption Fine Structure (*NEXAFS)* spectroscopy that allows the full and effective characterization of these types of devices [1-4].

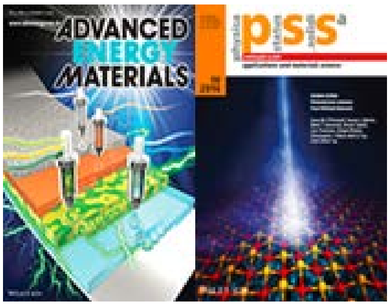

Figure 12 Studies of (a) solution processed organic semiconductors [1], and (b) functionalized electronic surfaces.

Soft X-ray spectroscopy at the Australian Synchrotron (in particular synchrotron based X-ray photoelectron spectroscopy) is being widely used as a highly effective tool to probe structure-function relationships in nanoscale electronic devices based on graphene [5-6] or diamond surfaces [7-8]. The beamline allows for the deposition and functionalization of a wide range of surfaces, as well as in situ characterization of properties such as the electronic work function.

1. Jung S., et al., All-Inkjet-Printed, *All-Air-Processed Solar Cells*, Advanced Energy Materials, 2014. **4**, p. 1400432
2. Deshmukh, K. et al., *Performance, morphology and photophysics of high open-circuit voltage, low band gap all-polymer solar cells*, Energy and Environmental Science, 2015. **8**: p. 332-342.
3. Huang, W. et al., *Unraveling the Morphology of High Efficiency Polymer Solar Cells Based on the Donor Polymer PBDTTT-EFT,* Advanced Energy Materials, 2015. **5**: p. 1401259.
4. Huang, W. et al., *In-depth understanding of the morphology-performance relationship in polymer solar cells*, Applied Materials and Interfaces, 2015. **7**: p. 14026–14034.
5. Cervenka, J. et al., *Graphene field effect transistor as a probe of electronic structure and charge transfer at organic molecule-graphene interfaces*, Nanoscale, 2015. **7**: p. 1471-1478.
6. Dontschu, N. et al., *A graphene field effect transistor as a molecule-specific probe of DNA nucleobases*, Nature Communications 2015. **6**: p. 6563.
7. O'Donnell, K. M., et al., *Extremely high negative electron affinity of diamond via magnesium adsorption*, Physical Review B 2015. **92**: p. 035303.
8. Stacey, A. et al., *Nitrogen Terminated Diamond*, Applied Materials Interfaces, 2015. **2**: p. 1500079.

Dr Eliot Gann

Australian Synchrotron and Monash University

Dr Gann is a Postdoctoral Fellow, jointly appointed with the Soft X-ray Beamline team at the Australian Synchrotron and with Assoc. Prof. Chris McNeill at Monash University.

Dr Gann and colleagues have had a wonderful couple of years, having published 16 papers containing Australian Synchrotron data (and others from elsewhere) in 2014 and 2015: *Journal of the American Chemical Society*, *Advanced Functional* and *Advanced Energy Materials*, *Nature Communications* & others…

Computational studies on materials for lithium and sodium ion batteries

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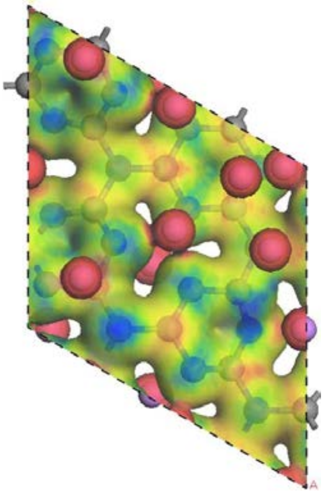

Graphite is the most commonly used anode material in commercialized lithium ion batteries due to its low cost and high chemical stability. It has many features that make it suitable for this application, such as low and flat voltage range, high Coulombic efficiency, good cyclability, low cost, and a small volume change on Li insertion. Two-dimensional (2D) graphene sheets can store Li on both sides giving rise to a theoretical capacity of LiC_3, which is larger than graphite. Graphene also has a large surface area, excellent electrical conductivity, and high chemical and thermal stability, making it seem suitable as an alternative material. However, at high loadings there it is predicted that the interaction mechanism changes, which is expected to result in low mobility. Therefore demand for higher capacity materials, graphene-like membranes or doped materials have been considered.

We have studied a range of carbon and carbon nitride materials for application as anodes in rechargeable batteries. In this talk, results from density functional theory calculations of the lithium and sodium adsorption and diffusion on 2D graphitic carbon and carbon nitride membranes will be presented. High-capacity Li storage has been predicted on graphdiyne [1] and has been confirmed experimentally. [2] In contrast we have found that high lithium adsorption energies on some carbon nitrides (C_3N_4 and C_6N_8 and bulk C_3N_4) results in severe distortion of the membrane or bulk material. This is shown to be consistent with experimental results on the charge and discharge capacities. [3]

1. Sun, C. and Searles, D.J., *Lithium Storage on Graphdiyne Predicted by DFT Calculations.* Journal of Physical Chemistry C, 2012. **116**: p. 26222-26226.
2. Huang, C., Zhang, S., Liu, H., Li, Y., Cui, G. and Li, Y. *Graphdiyne for high capacity and long-life lithium storage*. Nano Energy, 2015. **11**: 481–489.
3. Hankel, M., Ye, D. Wang, L. and Searles, D.J., *Lithium and Sodium Storage on Graphitic Carbon Nitride.* Journal of Physical Chemistry C, 2015. DOI: 10.1021/acs.jpcc.5b07572.

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School of Chemistry and Molecular Biosciences, The University of Queensland, Brisbane, Qld 4072 – Australia

Debra Bernhardt is recognised for her contributions to nonequilibrium statistical mechanics and thermodynamics including nonequilibrium and confined fluids. Her research involves a range of theoretical and computational approaches to develop a fundamental understanding of matter and study applications including transport in nanopores, fluctuations, material design, gas separation, and sustainable energy.

Dynamic Efficiency of Metallic Nanocatalysts

Hector Barron

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It is well established that the most efficient catalysts for all industrially relevant catalytic reactions (such as catalytic converters in the automotive industry, or electrochemical fuel cells), are Pt and Pd based nanostructures [1]. There is currently a significant global investment in developing more efficient Pt and Pd nanocatalysts, based on various strategies of structure/property engineering. The size, shape, and composition dependent efficiency is relatively well understood. However, no attention has been give to the other important parameter in determining the effectiveness of a catalyst: time. Time---dependence, in the form of growth rates, is one of the most important aspects of targeted synthesis, as knowing how fast to grow nanostructures (and when to stop growing) largely determines the amount and type of surfaces available for catalysis. Pt and Pd nanostructures that grow at different rates can end up having very different catalytic properties.

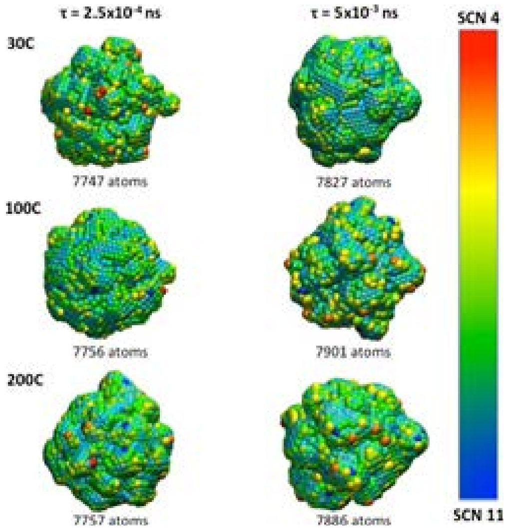

Fig.1. Final morphologies obtained at the end of the simulations and their surface coordination number (SCN). Lower coordinated atoms are localized on the tips and along the branches while higher coordinated atoms occupy "flat" areas over the surface

Moreover, the long---term time---dependent evolution, and the aging of nanostructured catalysts, determines their functional lifetime, and therefore the return on investment. Time-dependent performance determines economic efficiency [2].

In this work we model the time--- dependent evolution of the catalytic active sites (surface defects) to determine the efficiency in terms of their growth rates and temperatures. These results will guide experimental development, facilitate performance tracking, and the design of novel nanocatalysts.

1. Barnard, A. S. and Chang, L. Y. *Thermodynamic Cartography and Structure/Property Mapping of Commercial Platinum Catalysts*. ACS Catalysis, 2011. **1** (2): p. 76

2. Barron, H. and Barnard, A. S. *Using structural diversity to tune the catalytic performance of Pt nanoparticle ensembles*. Catal. Sci. Technol. 2015. DOI: 10.1039/c5cy00123d

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Dr. Hector Barron-Escobar was born in Mexico City where he attended National University of Mexico (UNAM) from 2000-2005 receiving a B.A. in Physics. After that he joined the Materials Research Institute (IIM) at UNAM where he received his M.S. in science materials and engineering. During his time at IIM he performed ab initio DFT calculations to amorphized crystalline cells of carbon. In 2008, Hector joined the Physics Ph.D. program at The University of Texas at San Antonio and began his work in Dr. Yacaman's group. During this time his work included the atomistic modeling of metallic NPs and the study of their energetic stability. In the summer of 2011 he joined the Laboratory of Computational Nanotechnology (LCNT) at The University of Texas at San Antonio, performing DFT calculations to study the structural, electronic and magnetic properties of bimetallic NPs, and the adsorption of methyl-thiol molecules on metallic clusters. In 2014 he was awarded with the OCE Postdoctoral Fellowship at CSIRO where he perform Molecular Dynamics (MD) computer simulations to design noble nanocatalysts based on Pt and Pd nanostructures, under the supervision of Dr. Amanda Barnard.

Mechanical Tensile Properties of Layered Sodium Titanate Nanowire

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Recently, ternary layered oxides like sodium titanate nanowire ($Na2Ti3O7$ NWs) is emerging as strong competitor in various fields due to their unique layered structure and structural versatility.[1] Notably, however, their structure-mechanical property relations are poorly studied and understood. In this work, we carried out a quantitative investigation on mechanical properties of hydrothermally synthesized $Na2Ti3O7$ NWs via *in situ* transmission electron microscope (TEM) uniaxial tensile testing under the assistance of a push-to-pull (PTP) device (Fig. 1a). We discovered that the $Na2Ti3O7$ NW exhibits a typical brittle behaviour with uniform square break point. The Young's modulus of the NW increases as the equivalent diameter of the NW decreases, ranging from 37 GPa to 185 GPa. These experimental values agree with the theoretical predictions based on density function theory (DFT) which provides guidance in its engineering applications. Interestingly, a wide range of reversible dislocation motion was observed after NW fracture (Fig. 1b). This highlighted a time-dependent recovery of the material even when the equivalent NW diameter is as large as 250 nm. The dislocation motion observation suggests anelastic property of $Na2Ti3O7$ NW which is further proved from a cantilever bending-relaxation test. The $Na2Ti3O7$ NW anelasticity is anticipated to be an external expression of stress-gradient-induced defect/dislocation migration.[2] Overall, we predict $Na2Ti3O7$ NW represented ternary layered oxides to be potential damping materials which also have wide space of various applications based on their outstanding mechanical property and great extent of structural tailorability.

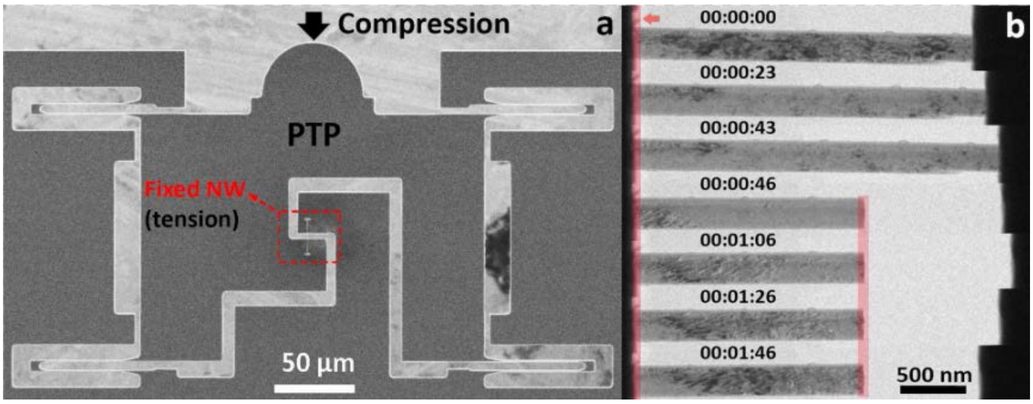

Fig. 1. a, SEM image of a PTP device where a fixed NW is bridged across the centre trench. b, images extracted from a movie of Na2Ti3O7 NW under tensile failure. Red arrow points out a stable feature on the PTP which is aligned by the longred transparent line. Short transparent line aligns the NW broken end.

[1] Kordás, K., et al., *Layered titanate nanostructures: perspectives for industrial exploitation.* Translational Materials Research, 2015. **2**(1): p. 0150031-18.

[2] Cheng, G., et al., *Large anelasticity and associated energy dissipation in single-crystalline nanowires.* Nature nanotechnology, 2015. **10**(8): p. 687-691.

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Dr. YuanTong Gu is now a Professor, a prestigious ARC Future Fellow and Discipline Leader at School of Chemistry, Physics and Mechanical Engineering of Queensland University of Technology (QUT). His research interests include Nanomaterial and Mechanical Engineering, Computational mechanics, and Biomechanics. He has secured 10 ARC grants with more than A$6million in research funding. He authored more than 180 refereed journal publications and one popular book. Most of his publications are in highly ranked journals and have been well cited. His expertise has been acknowledged through appointments as Editor-in-Chief for two international journals including Australian Journal of Mechanical Engineering, Associate Editor for a prestigious journal, Engineering Analysis with Boundary Elements, and an Editorial Board Member for another three SCI journals (Applied Mathematical Modelling, International Journal of Computational Methods, Multibody System Dynamics). He served as the conference general chair for the 4th International Conference on Computational Methods held at the Gold Coast in 2012. Currently, He is conference chair for The 2nd Australasian Conference on Computational Mechanics to be held at Brisbane in 2015.

Multifunctional materials for electronics and photonics

Federico Rosei

UNESCO Chair in Materials and Technologies for Energy Conversion, Saving and Storage

Centre for Energy, Materials and Telecommunications, INRS, 1650 Boul. Lionel Boulet, J3X 1S2 Varennes (QC), Canada

The bottom–up approach is considered a potential alternative for low cost manufacturing of nanostructured materials [1]. It is based on the concept of self–assembly of nanostructures on a substrate, and is emerging as an alternative paradigm for traditional top down fabrication used in the semiconductor industry. We demonstrate various strategies to control nanostructure assembly (both organic and inorganic) at the nanoscale. We study, in particular, multifunctional materials, namely materials that exhibit more than one functionality, and structure/property relationships in such systems, including for example: (i) control of size and luminescence properties of semiconductor nanostructures, synthesized by reactive laser ablation [2]; (ii) we developed new experimental tools and comparison with simulations are presented to gain atomic scale insight into the surface processes that govern nucleation, growth and assembly [3-7]; (iii) we devised new strategies for synthesizing multifunctional nanoscale materials to be used for electronics and photovoltaics [8-25].

References

[1] F. Rosei, *J. Phys. Cond. Matt.* **16**, S1373 (2004); [2] D. Riabinina, C. Durand, J. Margot, M. Chaker, G.A. Botton, F. Rosei, *Phys. Rev. B* **74,** 075334 (2006); [3] K. Dunn, J. Derr, T. Johnston, M. Chaker, F. Rosei, *Phys. Rev. B* **80**, 035330 (2009); [4] F. Ratto et al., *Small* **2**, 401 (2006); [5] F. Ratto et al., *Phys. Rev. Lett.* **96**, 096193 (2006); [6] F. Ratto, S. Heun, O. Moutanabbir, F. Rosei, *Nanotechnology* **19**, 265703 (2008); [7] F. Ratto, T.W. Johnston, S. Heun, F. Rosei, *Surf. Sci.*, **602**, 249 (2008); [8] F. Ratto, F. Rosei, *Mater. Sci. Eng. R* **70**, 243 (2010); [9] O. Moutanabbir, F. Ratto, S.

Heun, K. Scheerschmidt, A. Locatelli, F. Rosei, *Phys. Rev. B* **85**, 201416 (2012); [10] C. Yan et al., *Adv. Mater.* **22**, 1741 (2010); [11] C. Yan et al., *J. Am. Chem. Soc.* **132**, 8868 (2010); [12] R. Nechache et al., *Adv. Mater.* **23**, 1724–1729 (2011); [13] R. Nechache, C. Harnagea, S. Licoccia, E. Traversa, A. Ruediger, A. Pignolet, F. Rosei, *Appl. Phys. Lett.* **98**, 202902 (2011); [14] B. Aïssa, R. Nechache, D. Therriault, F. Rosei, M. Nedil*, Appl. Phys. Lett.* **99**, 183505 (2011); [15] G. Chen et al., D. Ma, *Chem. Commun.* **47**, 6308 (2011); [16] G. Chen, S. Desinan, R. Rosei, F. Rosei, D. Ma, *Chem. Comm.* **48**, 8009–8011 (2012); [17] G. Chen, F. Rosei, D. Ma, *Adv. Func. Mater.* **22**, 3914–3920 (2012); [18] R. Nechache, C. Harnagea, F. Rosei, *Nanoscale* **4**, 5588–5592 (2012); [19] S. Li et al., *Appl. Phys. Lett.* **101**, 192903 (2012); [20] J. Toster et al., *Nanoscale* **5**, 873–876 (2013); [21] T. Dembele et al., *J. Power Sources* **233**, 93–97 (2013); [22] S. Li et al., *Chem. Comm.* **49**, 5856–5858 (2013); [23] T. Dembele et al., *J. Phys. Chem. C* **117**, 14510–14517 (2013); [24] S. Li et al., *J. Am. Cer. Soc.* **96**, 3155 (2013); [25] R. Nechache et al., *Nature Photonics* **9**, 61 (2015).

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Federico Rosei has held the Canada Research Chair in Nanostructured Organic and Inorganic Materials since 2003. He is Professor and Director of Institut National de la Recherche Scientifique, Énergie, Matériaux et Télécommunications, Université du Québec, Varennes (QC) Canada. Since January 2014 he holds the UNESCO Chair in Materials and Technologies for Energy Conversion, Saving and Storage. He received MSc and PhD degrees from the University of Rome "La Sapienza" in 1996 and 2001, respectively.

Dr. Rosei's research interests focus on the properties of nanostructured materials, and on how to control their size, shape, composition, stability and positioning when grown on suitable substrates. He has extensive experience in fabricating, processing and characterizing inorganic, organic and biocompatible nanomaterials. He has published over **200** articles in prestigious international journals (including *Science*, *Nature Photonics*, *Proceedings of the National Academy of Sciences*, *Advanced Materials*, *Angewandte Chemie* Int. Ed., *Journal of the American Chemical Society*, *Advanced Functional Materials*, *Nanoletters*, *ACS Nano*, *Biomaterials*, *Small*, *Physical Review Letters*, *Nanoscale*, *Chem. Comm.*, *Applied Physics Letters*, *Physical Review B*, etc.), has been invited to speak at over **200** international conferences and has given over **170** seminars and colloquia and **20** public lectures in **42** countries on all inhabited continents. His publications have been cited over **5800** times and his H index is **41**.

In 2014, he has been elected Fellow of the Royal Society of Canada. He is Member of the European Academy of Sciences, Fellow of the American Physical Society, Fellow of the American Association for the Advancement of Science, Fellow of SPIE, Fellow of the Canadian Academy of Engineering, Fellow of ASM International, Fellow of the Royal Society of Chemistry (UK), Fellow of the Institute of Physics, Fellow of the Institution of Engineering and Technology, Fellow of the Institute of Materials, Metallurgy and Mining, Fellow of the Institute of Nanotechnology, Senior Member of the IEEE, Fellow of the Engineering Institute of Canada, Member of the Global Young Academy, Fellow of the Australian Institute of Physics and Member of the Sigma Xi Society.

He has received several awards, including the FQRNT Strategic Professorship (2002–2007), the Tan Chin Tuan visiting Fellowship (NTU 2008), the Senior Gledden Visiting Fellowship (UWA 2009), Professor at Large at UWA (2010–2012), a Marie Curie Post-Doctoral Fellowship from the European Union (2001), a Canada Research Chair since 2003 (renewed in 2008 for a second five year term) a Friedrich Wilhelm Bessel Award from the Alexander von Humboldt foundation (2011), the Rutherford Memorial Medal in Chemistry from the Royal Society of Canada (2011), the Herzberg Medal from the Canadian Association of Physics (2013), the Brian Ives lectureship award from ASM international / Canada Council (2013), the Award for Excellence in Materials Chemistry from the Canadian Society for Chemistry (2014), the NSERC EWR Steacie Memorial Fellowship (2014), the José Vasconcelos Award for Education from the World Cultural Council (2014), the IEEE NTC Distinguished Lectureship 2015, the Lash Miller Award from the Canada Section of the Electrochemical Society, the Chang Jiang Scholar Award from the Government of China, the Khwarizmi International Award (2nd Prize) from the Iran Research Organization for Science and Technology (IROST) and the Recognition for Excellence in Leadership from the American Vacuum Society.

Designing semiconducting metal oxides for solar energy conversion

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The capability of designing functional nanomaterials with desirable structures and properties remains an important challenge to R&D sectors. In this talk, we will give a brief overview on our recent progresses in designing layered semiconductor metal oxides materials for photoelectrochemical energy conversion including photocatalytic solar fuel generation and low cost solar cells. In more details, we have been focusing the following two aspects; 1) band-gap engineering of layered semiconductor compounds including layered titanate, tantalate and niobate-based pervoskites for visible light phtocatalysis, and 2) exfoliated nanosheets as building blocks for new photoelectrode design. The resultant material systems exhibited efficient visible light photocatalytic performance and improved power conversion efficiency, which underpin important solar-energy conversion applications including low cost solar cells and solar fuel production.

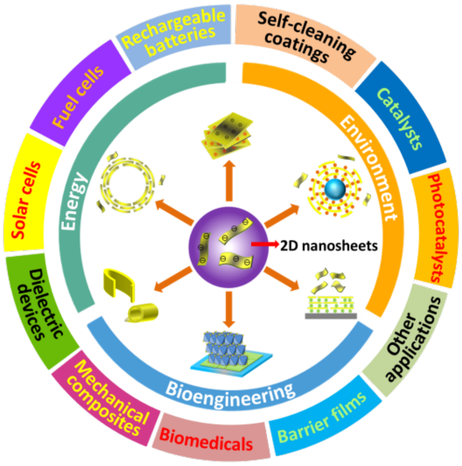

Figure 1. Schematic illustration of the use of exfoliated nanosheets as building blocks for new nanostructure design.[1]

Reference: 1. Wang & Sasaki, Chem. Rev., 2014, *114* (19), pp 9455–9486

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Lianzhou Wang is currently Professor in School of Chemical Engineering and Director of Nanomaterials Centre, the University of Queensland. He received his PhD degree from Shanghai Institute of Ceramics, Chinese Academy of Sciences in 1999. Before joining UQ in 2004, he has worked at two leading national research institutions (National Institute for Material Science and National Institute of Advanced Industrial Science and Technology) of Japan as a research fellow for five years. Since joining UQ, he has worked as Australian Research Council (ARC) Queen Elizabeth II Fellow (2006), Senior Lecturer (2007), Associate Professor (2010), and Professor (2012-) in School of Chemical Engineering and Affiliated Group Leader of Australian Institute for Bioengineering and Nanotechnology, UQ.

Lianzhou's research focuses on the synthesis, characterisation and application of functional nanomaterials for use in renewable energy conversion/storage systems, including photocatalytsts, low cost solar cells, rechargeable batteries, and water treatment membranes. In the last six years' time, as a Chief Investigator, he has succeeded in winning a large number of competitive grants, including 15 ARC grants and >10 research projects from other agencies such as CSIRO, Queensland Government, Corporative Research Centre, and UQ, totalling the funding of excess $15 million Australian dollars. Lianzhou has contributed 8 book chapters, >200 original journal publications (including top ranking journals such as *Chem Rev., Chem. Soc. Rev., Angew. Chem., Adv. Mater., J. Am Chem. Soc*., etc.), 11 patents and over 50 plenary/keynote/invited presentations, which received >6100 citations (Scopus). He has been actively involved in organising more than 25conferences and is severing as Associate Editor of *Journal of*

Nanoparticle Research and *Science Bulletin* and is also on Editorial Broad of three other international journals. Lianzhou has won some prestigious Fellowships/awards including STA Fellowship of Japan, ARC Queen Elizabeth II Fellowship (2006), UQ Research Excellence Award of 2008, Scopus Young Researcher Award of 2011 (Engineering and Technology category, Australian Universities), and ARC Future Fellowship of 2012.

Nanoengineered TiO_2 and Ta-doped TiO_2 for highly conducting transparent electrodes / functional photoanodes

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In this work we show and discuss the possibility of tuning electrical and optical properties of TiO_2 and Ta-doped TiO_2 (TaTO) thin films by engineering their nanoscale morphology and structure. TaTO belongs to a promising new class of recently discovered Transparent Conducting Oxides (TCO) [1,2], which are interesting because of the particular properties of TiO_2, such as its high chemical stability in a reducing atmosphere. Moreover, the usual employment of TiO_2 as an electron selective layer and photoanode in dye sensitized or perovskite-based solar cells motivates the study of the functional properties control in these TiO_2-based materials.

Here, amorphous TaTO films were deposited at room temperature via pulsed laser deposition in a background O_2 atmosphere, followed by thermal annealing to obtain polycrystalline anatase, while undoped TiO_2 was deposited for comparison. The best functional properties (resistivity ~5×10^{-4} Ωcm, mean transmittance in visible range exceeding 80% for a 150 nm thick TaTO film) were obtained when depositing with an oxygen pressure of 1 Pa followed by vacuum annealing at 550°C [3]. A thorough investigation of material properties was performed (X-ray diffraction, Raman spectroscopy, positron annihilation spectroscopy), with the aim of addressing the role of microstructure and defect chemistry on the functional properties of the material.

Notably, we demonstrate also the possibility to crystallize the films exploiting an ultra- fast thermal treatment at 460°C (ramp 300°C/min), by monitoring the crystallization threshold of the films via in-situ electrical measurements. This process not only reduces the annealing time down to a few minutes, but also provides the possibility to uncouple the electrical properties from the influence of the annealing environment. Remarkably, fast crystallization at ambient pressure in N_2 yields virtually the same conductivity as a conventional anneal carried out in vacuum (for doped and undoped TiO_2).

Finally, by increasing the O_2 pressure during the deposition process we are able to obtain tree-like nanostructured mesoporous layers, characterized by a large surface area, which could effectively act as photoanodes with tunable functional properties [4]. This opens the way to the realization of an all-TiO_2 transparent electrode/selective layer/photoanode, with a reduced number of interfaces and thus of recombination centers, which could be beneficial for electron transport.

1. Y. Furubayashi *et al*.. Appl. Phys. Lett. 86, 252101 (2005)
2. T. Hitosugi *et al*., Jap. J. Appl. Phys. 44, L1063 (2005)
3. P. Mazzolini *et al*., J. Phys. Chem C 119, 6988 (2015)
4. L. Passoni *et al*., ACS Nano 7, 10023 (2013)

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Born in Varese, Italy, 1972. 1997: master degree summa cum laude in Nuclear Engineering, Politecnico di Milano (Italy); 2000: Ph.D. in Condensed Matter Physics, Durham University (UK), with the thesis "X-ray and light scattering from nanostructured thin films". From 2002 to 2010 assistant professor and since 2010 associate professor of Physics of Matter at Politecnico di Milano, Department of Energy; 2013: National Scientific Qualification for full professor position.

He currently lectures Introduction to Nantechnology and Nanomaterials for Energy Conversion. He is responsible of the teaching and research activities of the Micro and Nanostructured Materials Laboratory; his current research interests concern the synthesis of nanostructured functional surfaces for energy applications; the investigation of model nanostructures and nanostructured surfaces by Scanning Tunneling Microscopy and Spectroscopy (STM/STS); the characterization of carbon-based and metal oxide nanostructured systems by Raman scattering. He is author of more than 100 scientific papers on peer reviewed journals (h-index ISI = 28, GoogleScholar = 32; for a list of publications see www.researcherid.com/rid/B-2448-2009). He has presented invited contributions to several international conferences and is referee of international journals, among which Physical Review B, Physical Review Letters, Applied Physics Letters. He has been coordinator of 7 research projects and responsible of research contracts with industrial partners. He is associated to the Center for Nano Science and Technology (CNST) of the Italian Institute of Technology at Politecnico di Milano (CNST-IIT@PoliMI), and member of the MIUR Center of Excellence for NanoEngineered Materials and Surfaces (NEMAS).

Plasmonic effects in photocatalysis: nanostructures for light absorption

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Photocatalytic processes offer the potential of utilizing the energy of photons to drive various useful chemical reactions including water purification [1] solar production of chemical feedstocks and fuels [2]. One approach to increase the efficiency of the photoconversion processes consists on integrating plasmonic metal nanostructures with semiconductor materials.

Plasmonic nanostructures can improve photocatalytic processes via: (i) intrinsic charge separation mechanisms (built- in potentials) that occur at metal–semiconductor junctions (Schottky contacts), (ii) strong confinement of electromagnetic energy at the surface of the metal nanoparticles, which leads to enormous energy densities at the near-field regions of the metallic nanostructures and (iii) the emission of hot charge–carriers from the metal nanoparticles into the semiconductor material.

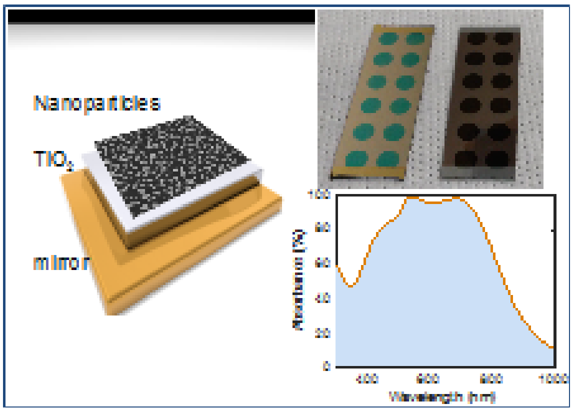

Figure 13: Plasmonic Super-absorbers for photocatalysis. **Left**: Diagram of the structures. **Upper right**: Fabricated structures using simple and inexpensive physical vapour deposition techniques. The dots are the super-absorber areas. **Bottom Right**: Measured absorbance spectrum demonstrating high broadband light absorption by a device that is only c.a. 40 nm in thickness.

The transfer of hot charge–carriers from metal nanostructures into photocatalytically active materials has recently been shown to be an efficient photocatalytic mechanism. This process is secondary to the initial step of *light absorption by the metal nanostructures*. Light absorption in these structures can be controlled by designing complex geometries with tailored optical cross-sections.

In this talk I will describe our approach to creating plasmonic structures for optimum absorption of light and generation of hot charge carriers. In particular, I will illustrate how we have employed concepts such as diffraction coupling in nanowire gratings [3] and nanorod dimer gratings [4] for achieving enhanced absorption. Additionally I will describe how we have employed simple interference effects in multilayered structures for achieving near perfect absorption of light in the visible (see figure 1.) in photoelectrochemical systems [5].

1. D. Bahnemann, Sol. Energy 2004, 77, 445.
2. D. M. Schultz, T. P. Yoon, Science 2014, 343, 1239176.
3. Ng, C. et al Advanced Optical Materials, 2015. DOI: 10.1002/adom.201500157
4. Piot, A. et al Nanoscale 2015, **7**, 8294.
5. Ng, C. *et al* In preparation 2015.

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Daniel Gomez completed a PhD in Chemistry at the University of Melbourne, under the supervision of Laureate Prof Paul Mulvaney in 2007, where he studied the optical properties of individual semiconductor nanocrystals. This work was then awarded the Chancellors Price for Excellence in the PhD Thesis in 2008. After a Post-Doc in CSIRO with Dr Timothy Davis where he studied the surface plasmon resonance of interacting nanoparticles, he was awarded the ARC Fellowship. He is an ARC Future Fellow at CSIRO working on applications of plasmonics in photochemistry.

Clusters for Photocatalysis

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Gold clusters with a size < 1.5 - 2 nm deposited on immobilized onto inert supports are known to be catalytic active with the size threshold often coinciding with the loss of metallic properties of Au nanoparticles The size-threshold is established for both naked clusters prepared under UHV conditions [1] and chemically-synthesised [2] well-defined metal nanoparticles. Clusters can be deposited from the gas phase as size selected clusters [3] or from the liquid phase when using chemically synthesised nanoparticles [4] with the latter route offering the benefit of easy scale-up.

In the deposition process of chemically made clusters onto inert supports a few challenges need to be solved. First, it needs to be investigated whether or not removal of the ligands is required to make the chemically made clusters catalytic active. The presence of ligands might hinder gas molecules to access the catalytic active sites of the clusters. We have found that removal of the phosphorous ligands can be achieved with heating to around 200ºC in vacuum [4]. Second, the agglomeration of the clusters needs to be avoided in order to keep the cluster size small. In particular heating for removal of the ligands could lead to agglomeration. We have deposited $Au_n(PPh_3)_y$ (n = 8, 9 and 101, y depending on the cluster size) on titania and found that treatment of the titania prior to deposition influences the agglomeration in the ligand removal process. Electron spectroscopy techniques (X-ray photoelectron spectroscopy (XPS)), scanning techniques (atomic force microscopy (AFM)) and microscopy ((scanning) transmission electron microscopy (STEM and TEM) have been used to investigate the deposition process. Subsequent to deposition also the electronic and conformational structure has to be determined because these are the two properties which are believed to play the crucial role for catalysis. Metastable induced electron spectroscopy (MIES) has been used for determining the electronic structure of deposited clusters.

References

[1] Valden, M.; Lai, X.; Goodman, D. W., *Onset of Catalytic Activity of Gold Clusters on Titania with the Appearance of Nonmetallic Properties*. Science, 1998. **281:** p. 1647-1650.

[2] Turner, M.; Golovko, V. B.; Vaughan, O. P. H.; Abdulkin, P.; Berenguer-Murcia, A.; Tikhov, M. S.; Johnson, B. F. G.; Lambert, R. M., *Selective Oxidation with Dioxygen by Gold Nanoparticle Catalysts Derived from 55-Atom Clusters.* Nature, 2008. **454**: p. 981-983.

[3] Büttner, M.; Oelhafen, P., *XPS Study on the Evaporation of Gold Submonolayers on Carbon Surfaces*. Surf. Sci. 2006. **600**:p. 1170-1177.

[4] Anderson, D. P.; Alvino, J. F.; Gentleman, A.; Qahtani, H. A.; Thomsen, L.; Polson, M. I. J.; Metha, G. F.; Golovko, V. B.; Andersson, G. G., *Chemically-Synthesised, Atomically-Precise Gold Clusters Deposited and Activated on Titania*. PCCP, 2013. **15**:p. 3917-3929.

Professor Gunther Andersson

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Gunther Andersson (born 1964) graduated from Dortmund University (Germany) in 1994. Soon after he started his PhD in a project on applying ion scattering spectroscopy on liquid surfaces at the University of Witten/Herdecke (Germany) under the supervision of Prof Harald Morgner. In 1998 Gunther completed his PhD and joined the research groups of Prof Hidde Brongersma and Martin de Voigt at the Eindhoven Technical University (The Netherlands). There he worked on a project on polymer based light emitting diodes. At the end of 2000 Gunther moved as Research Associate to the group of Prof Harald Morgner at Leipzig University (Germany) were he developed the method neutral impact collision ion scattering spectroscopy (NICISS) for investigation of soft matter surfaces to its current stage. He completed his Habilitation in 2006 and received his Venia Legendi. In 2007 he was appointed at Flinders University (Australia) as Senior Lecturer. He is currently leading as Associate Professor a research group with activities in liquid and polymer surfaces and catalysis based on nano-clusters.

Functional nanohybrids: plasma-related effects

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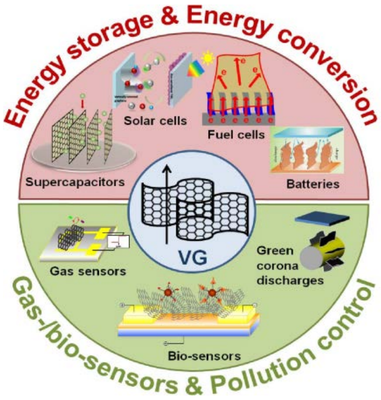
This presentation focuses on nanohybrid materials, such as carbon nanostructures decorated with oxide nanoparticles, oxide nanoparticles coated with organic nanofilms, and some others. In these cases effects related to low-temperature plasma treatments significantly improve the properties, stability, and performance of the nanohybrid materials.



In particular, the plasma processing of the surfaces of both organic and inorganic materials helps improving adhesion of the coated films or decorated nanoparticles. This usually results in better stability of the nano-composite structures in applications.

The applications involve harsh and strongly non-equilibrium conditions such as high-voltage electric stress in electrical insulation applications and chemically active solutions in electrochemical energy storage devices such as supercapacitors.

The high-voltage insulation nanocomposites are fabricated using plasma polymerization while hybrid supercapacitor electrodes are produced using plasma treatment of surfaces of carbon nanostructures. The interesting effects that arise due to the nanoscale plasma-surface interactions and the interesting properties of the nanostructures [1,2] in each case are discussed.

These interactions can be enabled by atmospheric-pressure plasma discharges thereby avoiding expensive vacuum systems and processes. Some of the applications of functional nano-hybrids based on vertical graphenes are summarized in the figure reproduced from Ref. [2].

[1] K. Ostrikov, E. C. Neyts, and M. Meyyappan, *Adv. Phys.* 62, 113 (2013)

[2] Z. Bo, S. Mao, Z. J. Han, K. F. Cen, J. H. Chen, and K. Ostrikov, *Chem. Soc. Rev.* 44, 2108 (2015)

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Kostya (Ken) Ostrikov is a CEO Science Leader, Australian Future Fellow (Professorial-Level (FT3) in Nanotechnology as the primary field of research), CSIRO's Chief Research Scientist in Plasma- and Nano- Technologies, and a Founding Leader of the Plasma Nanoscience Laboratories, Manufacturing Flagship, CSIRO, Professor of Nanotechnology and Molecular Science at the Faculty of Science and Engineering of Queensland University of Technology (QUT), and a Founding Leader of CSIRO-QUT Joint Sustainable Processes and Devices Laboratory (Sydney-Brisbane-Melbourne) and as well as an Honorary/Visiting Professor of the University of Sydney, University of Technology Sydney, University of Wollongong (Australia); Huazhong University of Science and Technology, Shanghai Jiaotong University, Jiangnan University (China); Kharkiv National University (Ukraine); Nanyang Technological University (Singapore); and Josef Stefan Institute (Slovenia, EU). He pioneered and developed the Plasma Nanoscience as a distinctive research field [Rev. Mod. Phys. 77, 489 (2005), IF=51.4 (2010), Australia's only paper in 8 years before publication] and has lead it to recognition as a major advance in physics [Adv. Phys. 62, 113 (2013) (IF=37.0, 2011); Australia's only 13-th paper in 62 years]. He is the only person in the world who published a solo paper in one of these (two highest-IF journals in physics at the time of publication) journals and a first-author paper in another one in last decade.

As an established and recognized leader of a large international collaborative network, convenor of annual conferences, and lead editor of special issues in the field, he leads a large international plasma nanoscience community. He is the first recipient of the high-profile 2012 Building Future Award of Germany's Ministry of Economics, Association of Electronic and Electrotechnical Industries, and the world's largest Trade Fair Messe Frankfurt *in recognition of outstanding achievements and innovations in scientific research that sets a landmark in sustainable development in our society.* His achievements include the 3 most prestigious general-field (physics) medals of National Academies of Science of Australia and Ukraine and the Australian Institute of Physics (*one of the only two researchers who have been awarded both of the two most prestigious medals in physics [AIP Walter Boas (2010) and AAS Pawsey (2008)] in Australia in last decade*), 7 prestigious international fellowships and 10 full professor-level appointments in 6 countries, 3 research monographs, nearly 450 refereed journal papers *(H-index of 54 has been achieved in only 17.5 career years, which is exceptional as it is 3 times higher than the accepted sign of success [Nature 436, 900 (2005)]) and is higher than his physical age*, more than 100 plenary, keynote, and invited talks at international conferences, research training of ~30 researchers with PhD and >60 research students, as well as more than $10M in competitive research funding and more than 200 coauthors/collaborators in last 5-6 years. Staff, postdocs, and students trained in CSIRO by Ostrikov are well-known and recognized nationally and internationally (e.g., prestigious fellowships, awards, publications, invitations, etc.). His research on *nanoscale control of energy and matter for a sustainable future* contributes to the solution of the grand challenge of directing energy and matter at the nanoscale, a challenge that is critical for renewable energy and energy-efficient technologies for a sustainable future.

Layer-by-Layer Assembly: Technologies and Applications

Joseph J. Richardson

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Methods for depositing multilayer thin films on planar and particulate substrates are important for generating functional materials capable of diverse applications. The repeated deposition of complementary polymers in a layer-by-layer (LbL) manner is a particularly promising method for depositing thin films as it allows for molecular-scale control over the film properties.[1]

LbL assembly can be as simple as dipping a substrate into polymer solutions in an alternating fashion, which has allowed LbL assembly to infiltrate most fields of research. Of course, more complex assembly methods exist, such as electrophoretic deposition, or spraying polymer solutions onto a rotating substrate, or even building up metal-organic frameworks one molecule at a time.[2]

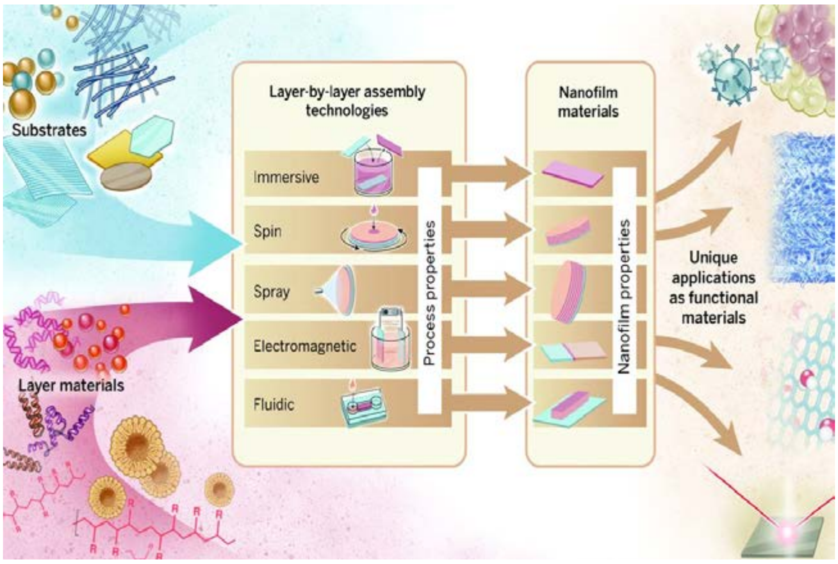

Figure 14. Layer-by-layer assembly [2]

In this lecture I will focus on different technologies useful for LbL assembly and explain the various applications that have arisen from LbL films.

The history of LbL can be traced back over 50 years, and in that time various technologies have evolved to prepare films for numerous applications. Primarily the technologies fall into 5 categories: immersive, spin, spray and electromagnetic assembly. These technologies have enabled diverse uses for LbL films include the coating of laser fusion targets and clothes, the formation of fire-resistant materials and sensors, the assembly of batteries and optical coatings, and the construction of films for various biomedical applications.[2] I will review some of these applications with an additional focus on novel LbL methods for coating particulate substrates.[3]

1. Decher, Gero. *Fuzzy nanoassemblies: toward layered polymeric multicomposites*. Science, 1997 **277**(5330): p. 1232.
2. Richardson, Joseph J., et al. *Technology-driven layer-by-layer assembly of nanofilms*. Science, 2015 **348**(6233): aaa2491.
3. Richardson, Joseph J., et al. *Preparation of Nano-and Microcapsules by Electrophoretic Polymer Assembly*. Angew. Chem. Int. Edit. 2013 **52**(25): p. 6455.

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Joseph J. Richardson has a unique perspective for materials research because of his diverse background, including degrees in Philosophy and Industrial & Systems Engineering. His thesis work under Prof. Frank Caruso at the University of Melbourne dealt with discovering new techniques for layer-by-layer assembly. During this time he also worked on the assembly of coordination stabilized films, and the application of thin films in biology and medicine. Currently he works at CSIRO under the guidance of Dr. Paolo Falcaro on hybrid Metal-Organic Frameworks for biomedical engineering.

Flame Synthesis of Tailored Nanostructures for Highly Performing Devices

Antonio Tricoli

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In the last two decades, nanomaterials have become a key building block of a rapidly increasing number of products and devices. Their application ranges from advanced nanocarriers for targeted drug delivery to nanocatalysts for artificial photosynthesis and energy storage. Widespread commercial exploitation of the unique properties of nanostructures requires scalable and low cost synthetic routes capable of providing accurate fine-tuning of composition and morphology as well as their reproducible assembly into hierarchical microstructures.

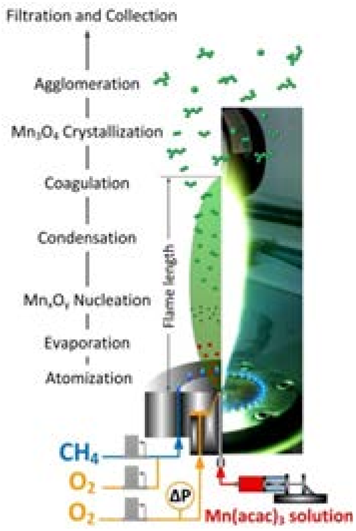

Figure 15 Flame synthesis of efficient water splitting nanocatalysts

Flame synthesis is a scalable low-cost approach currently utilized for the production of numerous nanoparticle commodities including carbon black, fumed silica and pigmentary titania.[1] Recently, the development of liquid-fed spray flames has greatly expanded their synthesis capabilities enabling the engineering of more complex nanostructures made of multi metal-oxides, core-shell morphologies and unique metastable phases[2]. Furthermore, their direct aerosol deposition from the gas phase offer a well-controlled approach for the fabrication of ultra-porous films with potential for numerous devices[2].

In this lecture, I will first introduce to the fundamentals of flame synthesis of nanostructures and aerosol self-assembly of ultra-porous hierarchical films. I will present a short review of the evolution of flame reactors and their current commercial applications. Thereafter, I will discuss some of the unique material structures that have been successfully synthesized by flames. Finally, I will emphasize some emerging applications of flame synthesis and aerosol deposition to the fabrication of highly performing photo- and chemical sensors for wearable device technology[3].

1. *Pratsinis, S.E., Flame Aerosol Synthesis of Ceramic Powders.* Progress in Energy and Combustion Science, 1998, **24**(3): p. 197-219.

2. Strobel, R. et al., *Flame aerosol synthesis of smart nanostructured materials.* Journal of Materials Chemistry, 2007, **17**(45): p. 4743-4756.

3. Nasiri, N. et al., *Ultraporous Electron-Depleted ZnO Nanoparticle Networks for Highly Sensitive Portable Visible-Blind UV Photodetectors*. Advanced Materials, 2015, 10.1002/adma.201501517.

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Antonio Tricoli received his master in Mechanical and Process Engineering from the Swiss Federal Institute of Technology (ETH Zurich) in 2004. Immediately after, he joined the Renewable Energy Laboratory of ETH Zurich where he worked on the production of solar hydrogen by two-step water splitting cycles. He continued his studies in 2005 at the Particle Technology Laboratory (ETH Zurich) researching the synthesis and self-assembly of nanoparticle films by combustion of organometallic precursors. In 2010, he received his PhD in the field of Nanotechnology focusing on the self-assembly of inorganic nanostructures for gas sensing. He further pursued his work as research fellow and lecturer at ETH Zurich focusing on the rapid synthesis of nanoparticle and nanowire layers for dye sensitized solar cells and non-invasive medical diagnostics. In 2012, he joined the Australian National University as research fellow under a five year Future Engineering Research Leadership Fellowship. Since then, he has founded the Nanotechnology Research Laboratory at the ANU and currently supervises several projects focusing on the synthesis of highly porous films made of tailored multi-layer inorganic nanostructures for integrated devices and on functionalization of advanced nanocomposites for regenerative medicine and medical diagnostics.

Conversion of n-Type CuTCNQ into p-Type Nitrogen-Doped CuO and the Implication for Room Temperature Gas Sensing

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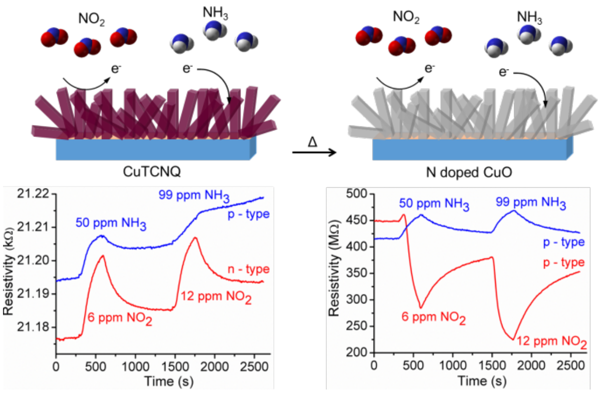
In this work, as-deposited and annealed microrods of semiconducting CuTCNQ (TCNQ=7,7,8,8-tetracyanoquinodimethane) with nanostructured features were evaluated for gas sensing towards NO_2 and NH_3 in the temperature range of 25˚-100°C. It was found that CuTCNQ is transformed into a N-doped CuO material with p-type conductivity when annealed at the maximum temperature of 200°C. This is the first time that such a transformation, from a semiconducting charge transfer material into a N-doped metal oxide is detected. This significantly enhanced the sensing response towards NO_2 and NH_3 gases compared to CuTCNQ. For the N-doped CuO sensor, a detection limit of 1 ppm for NO_2 and 10 ppm for NH_3 were achieved. This method opens up the possibility of using other MTCNQ sensing layers for room temperature gas sensing and their possible conversion to the N-doped metal oxide counterpart upon annealing.



Journal of Physical Chemistry C, 2015 (in press)

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Dr Mahnaz Shafiei received her bachelor of science in electrical and electronics engineering from AmirKabir University of Technology (Tehran Polytechnique), Iran. She completed her PhD at RMIT University, Australia in 2011. She is currently a Research Officer at QUT, Australia. She was awarded Endeavour Research Fellowship 2015 undertaking a research at Simon Fraser University, Canada. Her major area of research includes chemical sensors, nanotechnology and material sciences.

Vortex fluidics organisation of materials

Colin L Raston

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The presentation will highlight the application of a vortex fluidic device (VFD) [1] which generates intense shear within dynamic thin films, and can operate under continuous flow conditions or confined mode. Within these films nanomaterials can be fabricated in a precise way for both bottom up and top down approaches, and can be used to control the pore size and wall thickness of mesoporous materials, control folding of proteins, and control the phase of materials, the formation of graphene scrolls, slicing SWCNT and MWCNT < 400 nm, biodiesel production, organic reactions, and much more.

The thin film in VFD ensures uniform heat transfer and mixing, and surface Faraday waves break down the surface tensions and result in high mass transfer of gases. All molecules are treated in the same way, which can be varied by varying the VFD control parameters, including concentrations, temperature, flow rates, tilt angle θ, rotational speed, and surface contact angle, as well as using field effects (magnetic, pulsed laser and UV, plasma),

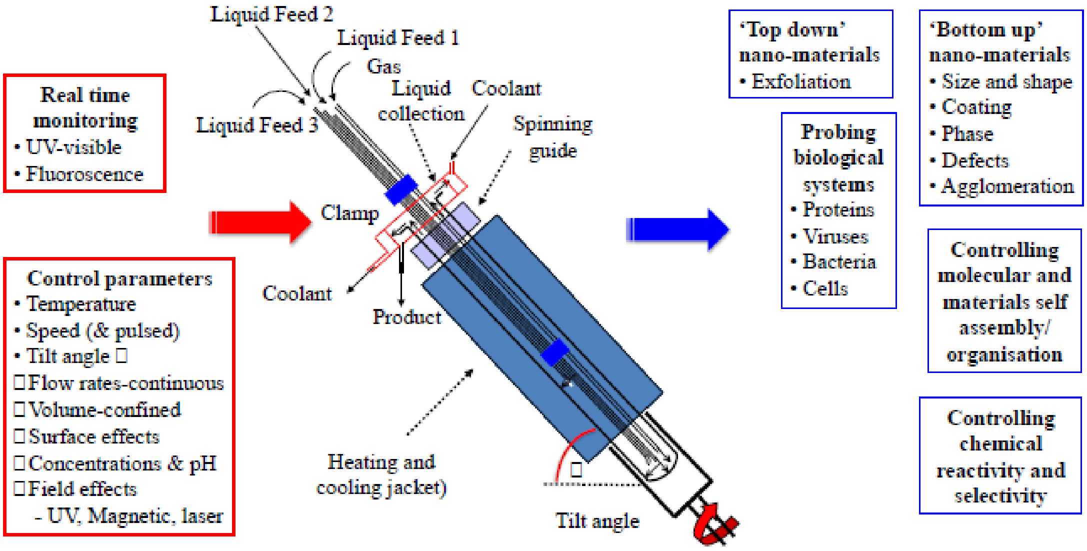

Figure 1: Diagram of the vortex fluidic device (VFD), highlighting the control parameters, which includes the use of field effects, and some of the potential applications.

References:

[1] L. Yasmin, X. Chen, K. Stubbs and C. L. Raston. "Optimising a vortex fluidic device for controlling chemical reactivity and selectivity" Sci. Rep. 2013, 3, 2282.

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Prof Colin Raston is a SA Premier's Professorial Research Fellow in Clean Technology, at Flinders University. He completed a PhD under the guidance of Professor Allan White, and after postdoctoral studies with Professor Michael Lappert (FRS) at the University of Sussex, he was appointed a lecturer at The University of Western Australia (1981) then to Chairs of Chemistry at Griffith University (1988), Monash University (1995), The University of Leeds (2001), and The University of Western Australia (2003). He is a former President, Queensland Branch President, and Chair of the Inorganic Division, the Royal Australian Chemical Institute (RACI). He has received the RACI's Green Chemistry Challenge Award, the H.G. Smith Award, the Burrows Award, and the Leighton Memorial Award, and is a former recipient of an ARC (Australian Research Council) Special Investigator Award, ARC Senior Research Fellowships and ARC Australian Professorial Fellowships. His current research covers clean technology and green chemistry, biomass processing, process intensification, nanotechnology and self-assembly, and is currently on the editorial advisory board of the international journal Green Chemistry, and on the editorial boards of Crystal Growth and Design and Polyhedron. Professor Raston has published over 700 journal articles, and has a book, chapters in books, and has patents on fullerene, nano-particles, calixarenes, carbon nanotube separation, microfluidics and surface technology.

Engineering Metal-Organic Frameworks

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Metal organic frameworks (MOFs) are a class of ultra-porous materials with exceptionally high accessible surface area and structure modularity due to the framework produced by the inorganic nodes coordinated by organic bridging ligands.[12,3]

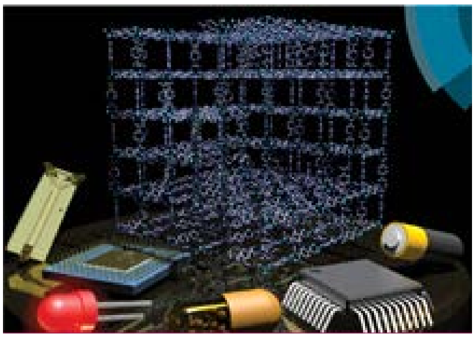

Figure 16 Illustration of different applications of Metal-Organic Frameworks

A number of increasing studies are investigating Metal-Organic Frameworks (MOFs) for a variety of functional applications including sensing, microelectronics, energy production, drug delivery and microfluidics.[4] However, MOF-based device fabrication requires synthetic protocols for the controlled functionalization of the ultra-porous crystals and their integration in suitable platforms.[4] This presentation will summarize the recent progress on MOF crystal engineering aspects, such as the functionalization of MOFs[5,6,7,8] and the controlled growth of MOFs on substrates.[9,10,11]

[1] Furukawa, H.; Cordova, K. E.; O'Keeffe, M.; Yaghi, O. M. *Science* **2013**, 341 (6149), 1230444.

[2] Guillerm, V.; Kim, D.; Eubank, J. F.; Luebke, R.; Liu, X.; Adil, K.; Lah, M. S.; Eddaoudi, M. *Chem. Soc. Rev.* **2014**, 43 (16), 6141–6172.

[3] Kitagawa, S.; Kitaura, R.; Noro, S. *Angew. Chem. Int. Ed.* **2004**, 43 (18), 2334–2375.

[4] Falcaro, P.; Ricco, R.; Doherty, C. M.; Liang, K.; Hill, A. J.; Styles, M. J. *Chem. Soc. Rev*. **2014**, 43 (16), 5513–5560.

[5] Doherty, C. M.; Buso, D.; Hill, A. J.; Furukawa, S.; Kitagawa, S.; Falcaro, P. *Acc. Chem. Res.* **2014**, 47 (2), 396–405.

[6] Zanchetta, E.; Malfatti, L.; Ricco, R.; Styles, M. J.; Lisi, F.; Coghlan, C. J.; Doonan, C. J.; Hill, A. J.; Brusatin, G.; Falcaro, P. *Chem. Mater.* **2015**, 27 (3), 690–699.

[7] Ricco, R.; Malfatti, L.; Takahashi, M.; Hill, A. J.; Falcaro, P. *J. Mater. Chem. A* **2013**, 1 (42), 13033–13045.

[8] Okada, K.; Ricco, R.; Tokudome, Y.; Styles, M. J.; Bell, S.; Kirby, N.; Mudie, S; Haylock, D.; Hill, A. J.; Doonan, J.; Falcaro, P. *Nat.Commun* **2015**, 6, 7240.

[9] Liang, K.; Ricco, R.; Doherty, C.M.; Styles, M. J.; Hill, A. J.; Takahashi, M.; Falcaro, P. *Adv. Funct. Mater.* **2014**, 24 (14), 1969–1977

[10] Toyao, T.; Liang, K.; Okada, K.; Ricco, R.; Styles, M. J.; Tokudome, Y.; Horiuchi, Y.; Hill, A. J.; Takahashi, M.; Matsuoka, M.; Falcaro, P. *Inorg Chem Front* **2015**, 2, 434.

[11] Liang, K.; Carbonell, C.; Styles, M.J.; Ricco, R.; Styles, M. J.; Jiwi, C.; Richardson, J.J.; Maspoch, D.; Caruso, F.; Falcaro, P. *Advanced Materials* **2015***, in press*.

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Paolo Falcaro holds a PhD in material engineering jointly awarded by Padova University and Bologna University in 2006. From 2005 to 2009 Paolo worked in a research company to develop/optimize industrial products. In 2009 he joined CSIRO extending the expertise from Sol-Gel and device fabrication to Metal-Organic Frameworks (MOFs). Paolo's research focuses in device fabrication using self-assembled materials for sensing, decontamination and bioprocessing. He is currently Team Leader of the Adaptive Porous Materials Team. Paolo published over 80 papers in international journals. He is guest professor at Osaka Prefecture University and Kyoto University (Japan).

Combined Raman, IR and DFT investigations of superconductivity in AlB_2-type and related structures

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Boron displays bonding characteristics that, in many respects, are similar to those of carbon. Boron forms a range of frameworks with a high degree of flexibility, within which a wide range of metal atoms are accommodated. This capacity to flex and to contain many metals results in a range of physical properties which do not invoke major changes in crystal structure[1, 2]. The refractory nature of many borides and limited choices for facile, low temperature processing suggests that the full potential of boron-based structures remains to be explored.

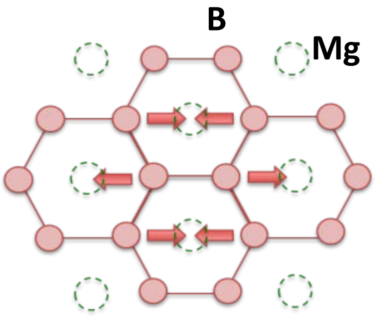

Figure 17: Magnesium diboride structure looking down the c axis.

Boride compounds predominantly display simple, high symmetry structures that, with metal substitution, result in a diversity of physical properties. We have used this feature of metal borides as test systems to compare experimental results with theoretical predictions[1-3]. While several examples of superconductivity can be found in boride chemistry, MgB_2 is the standout material with a superconducting transition temperature (T_c) of 39.5 K[4]. Other borides, such as YB_6, ThB_6 and mixed metal diborides[1, 2, 5] (e.g. $Mg_{0.7}Al_{0.3}B_2$) are also superconductors but with lower values for T_c. We have used DFT calculations to assess the electronic structures as well as phonon distributions for a wide range of metal borides and to compare these outcomes with key experimental parameters. We show that key experimental properties of metal borides can be correlated with DFT models, particularly with layered diboride structures as shown in Figure 1.

In our recent work[3, 6], observations of extra Raman and IR peaks in spectra from quality MgB_2 crystals led us to review explicit aspects of the generally accepted P6/mmm symmetry. Phonon dispersion (PD) calculations show that a viable explanation for Raman and Infrared results can be achieved by reducing the symmetry of the group determined from refinements of X-ray and neutron diffraction studies[7, 8]. A reduction in symmetry allows a better approximation to dynamical distortions induced in the boride system by the phonons themselves. Furthermore, inclusion of spin polarization leads to increased mathematical accuracy and improved physical interpretation of functional calculations especially for superconducting borides[2]. We show that a focus on PD calculations for diboride structures provides key insight into the electron-phonon coupling previously described by experimental data[9].

References:

1. I. D. R. Mackinnon, J. A. Alarco and P. C. Talbot, *Modelling & Numerical Simulation of Material Science*, 2013, **3**, p 158-169.
2. J. A. Alarco, P. C. Talbot and I. D. R. Mackinnon, *Modelling and Numerical Simulation of Material Science*, 2013, **4**, p 53-69.
3. J. A. Alarco, A. Chou, P. C. Talbot and I. D. R. Mackinnon, *Phys. Chem. Chem. Phys.*, 2014, **16**, p 24443-24456.
4. J. Nagamatsu, N. Nakagawa, T. Muranaka, Y. Zenitani and J. Akimitsu, *Nature*, 2001, **410**, p 63-64.

5. J. Y. Xiang, D. N. Zheng, J. Q. Li, L. Li, L. P. L. Lang, H. Chen, C. Dong, G. C. Che, Z. A. Ren, H. H. Qi, H. Y. Tian, Y. M. Ni and Z. X. Zhao, *Physical Review B*, 2002, **65**, p 214536-1-6.
6. J. A. Alarco, P. C. Talbot and I. D. R. Mackinnon, *Phys. Chem. Chem. Phys.*, 2014, **16**, p 25386-25392.
7. A. Q. R. Baron, H. Uchiyama, R. Heid, K. P. Bohnen, Y. Tanaka, S. Tsutsui, D. Ishikawa, S. Lee and S. Tajima, *Phys. Rev. B*, 2007, **75**, p 020505-1-4.
8. N. D. Markovskiy, J. A. Mu˜noz, M. S. Lucas, Chen W. Li, O. Delaire, M. B. Stone, L. Abernathy and B. Fultz, *Phys. Rev. B*, 2011, **83**, p 174301-174307.
9. J. Kortus, *Physica C*, 2007, **456**, p 54-62.

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Jose has an undergraduate degree in Physics from The National University of Engineering in Peru and a PhD in Materials Science from Chalmers University of Technology in Sweden. He has been involved in R&D on superconductors, battery and other nanotechnology materials for almost two decades, both within academic and commercial organizations. He has co-developed and holds numerous patents in generic processes for the manufacture of nano-scale complex, metal oxides and for applications in catalysis, batteries, electronics, etc. His current R&D interests include the synthesis of new compounds, physical property measurements and comparison with DFT calculations, with the aim to use DFT as a predictive tool for new compounds with enhanced properties.

Energetics of nano-layer structures from semi-analytic RPA-level theory

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Sebastien Lebegue

CNRS and University of Lorraine, France

Systems consisting of nanothin layers, such as multilayer structures and their adsorbates, are often bound largely by dispersion (van der Waals, vdW) forces, so that semi-local energy functionals are not adequate for modeling them. Much recent effort has therefore been put into simple vdW corrections, most typically involving a pairwise atom-based sum of vdw-type R^{-6} atom-atom interactions. Some more sophisticated (vdW-DF) theories also can be expressed via pairwise summation. While such pairwise approaches are computationally efficient and often have good success with the inner, close-contact parts of the binding energy curves, it is known that they give an incorrect description of the more distant energetics, especially for layers that are highly polarizable, metallic or semi-metallic such as graphene. For these phenomena one needs the correlation energy at the Random Phase Approximation (RPA) level of accuracy, or beyond. RPA-based methods are computationally impractical for many interesting geometries, however.

Here we introduce a method, which we term Layer Response Theory, that reproduces semi-analytically the RPA energetics in the outer part of the energy-versus-separation curve. It is based on a relatively efficient computation of the long-wavelength electronic response of an isolated atomically thin layer, by analytically deconvoluting the layer interactions in a macroscopic dielectric function calculation for an infinite stack of layers that has been only slightly stretched. This then allows a very efficient RPA-type energy computation involving arbitrary layer structures and adsorbates.

Professor John Dobson

Queensland Micro and Nano Technology Centre, Griffith University, Australia

Professor John Dobson researches many-electron quantum physics and nanoscience in the Queensland Micro and Nano Technology Centre, and also teaches physics at all levels at Griffith University. He obtained his undergraduate degree at Melbourne University and his doctorate at the University of California. He has also worked at Cornell University (USA), University of Paris and Ecole Polytechnique (France).. His research area is condensed matter theory, and he has made contributions in recent years in the areas of time dependent Density Functional Theory, theory of dispersion (van der Waals) interactions, and properties graphene.