

**Imperial College
London**

DEPARTMENT OF CHEMICAL ENGINEERING

DEPARTMENT OF CHEMICAL ENGINEERING POSTDOC SYMPOSIUM 2015



23 SEPTEMBER 2015, 12:00–17:00

Talks in Lecture Theatre 1, (ACEX 250)

Poster presentations in the Level 3 Design rooms

PROGRAMME AND BOOK OF ABSTRACTS

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Organising committee

Academics: Cleo Kontoravdi, George Jackson

Postdoc representatives: Yolanda Sanchez-Vicente, Maria Jimenez Solomon, Peter Yatsyshin

Support staff: Zoe Townsend, Michael Panagopoulos

PROGRAMME

12:00–13:25 <i>Lunch and Poster session in Level 3 Design Rooms</i>		
13:30–14:10	Pinky Dua <i>Senior Director and Head of Clinical Pharmacology, Pfizer</i>	<i>Keynote lecture:</i> Modelling and simulation in drug discovery and development
14:10–14:30	Lisa Kleiminger	Closing the renewable energy gap – energy storage employing solid oxide electrolysers
14:30–14:50	Santanu Karan	Sub–10 nm polyamide nanofilms with ultrafast solvent transport for molecular separation
14:50–15:10	Alessandra Vitale	Coupling frontal photopolymerization and surface instabilities for a novel 3D patterning process
15:10–15:30 <i>Break</i>		
15:30–15:50	Qilei Song	Molecularly designed functional nanomaterials for energy and sustainability
15:50–16:10	Angelo Pomella	Understanding cell rupture mechanisms in ultrasonication for bioprocessing applications
16:10–16:30	Alex Brogan	Protein-polymer surfactant nanoconstructs for increased solubility and thermal stability in ionic liquids
16:30–16:55	James Kimber	<i>Sir William Wakeham Award lecture:</i> ATR-FTIR Spectroscopic imaging of dynamic processes
16:55–17:00 <i>Closing remarks & prizes</i>		
17:00–18:00 <i>Informal drinks in the SCR</i>		

SPEAKER ABSTRACTS

Closing the renewable energy gap – energy storage employing solid oxide electrolyzers

Lisa Kleiminger, N Farandos, T Li, GH Kelsall

14:10–14:30

l.kleiminger11@imperial.ac.uk

As renewable energy sources are inherently intermittent, their increasing contributions to electricity grids will necessitate large-scale energy storage to balance supply and demand. Storing electrical energy in chemical bonds by electrolysis of CO₂ and / or H₂O is one technology to achieve this. I chose solid oxide reactors for this application, as they can be operated cyclically in electrolyser (energy storage) and fuel cell (energy re-generation) modes.

A novel fabrication is presently being developed using 3-D ceramic ink-jet printing ('additive manufacturing') to print functional layers of these solid oxide reactors. This technology will eventually be employed to fabricate 'electrodes-by-design', enhancing reactor performance, as well as producing more geometrically reproducible structures to enable determination of micro-kinetic parameters required as inputs to finite element reactor models.

Results will be presented for 3-D printing of preliminary electrolyser structures. The concept of cyclic energy storage will be illustrated based on hollow fibre electrolyzers, previously developed within the department [1,2].

[1] L. Kleiminger, T. Li, K. Li and G.H. Kelsall, RSC Adv., 4 (2014) 50003-50016.

[2] L. Kleiminger, T. Li, K. Li and G.H. Kelsall, Electrochim. Acta, (2015) in press.

Sub-10 nm polyamide nanofilms with ultrafast solvent transport for molecular separation

Santanu Karan, Z Jiang, AG Livingston

14:30–14:50

skaran@imperial.ac.uk

Membranes with unprecedented solvent permeance and high retention of dissolved solutes are needed to reduce the energy consumed by separations in organic liquids. We used controlled interfacial polymerization to form free-standing polyamide nanofilms less than 10 nanometers in thickness, and incorporated them as separating layers in composite membranes. Manipulation of nanofilm morphology by control of interfacial reaction conditions enabled the creation of smooth or crumpled textures; the nanofilms were sufficiently rigid that the crumpled textures could withstand pressurized filtration, resulting in increased permeable area. Composite membranes comprising crumpled nanofilms on alumina supports provided high retention of solutes, with acetonitrile permeances up to 112 liters per square meter per hour per bar. This is more than two orders of magnitude higher than permeances of commercially available membranes with equivalent solute retention.

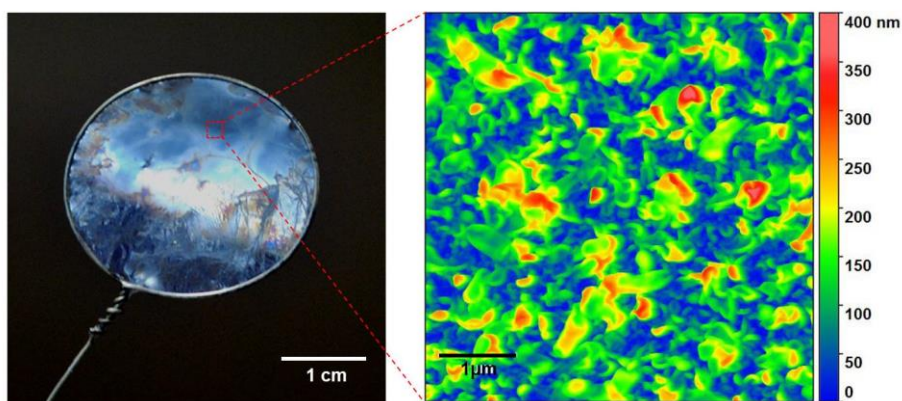


Figure 1. Freestanding sub-10 nm polyamide nanofilm on a lasso and the AFM image showing crumpled features.

References

1. Santanu Karan, Sadaki Samitsu, Xinsheng Peng, Keiji Kurashima and Izumi Ichinose, *Science*, 335, 444–447, 2012.
2. Patricia Gorgojo, Santanu Karan, H. C. Wong, M. F. Jimenez-Solomon, J. T. Cabral and Andrew G. Livingston, *Advanced Functional Materials*, 24, 4729–4737, 2014.
3. Santanu Karan, Zhiwei Jiang and Andrew G. Livingston, *Science*, 348, 1347–1351, 2015.

Coupling frontal photopolymerization and surface instabilities for a novel 3D patterning process

Alessandra Vitale, MG Hennessy, OK Matar, JT Cabral 14:50–15:10

a.vitale@imperial.ac.uk

Patterning of soft matter provides an exceptional route for the generation of micro/nanostructured and functional surfaces. We describe a new 3D fabrication process based on coupling frontal photopolymerization (FPP) with precisely controlled, yet spontaneous, interfacial wrinkling.

FPP is a complex spatio-temporal process that can lead to the formation of well-defined propagating fronts of network formation, both stable and unstable. We investigate this process focusing on the interfacial monomer-to-polymer conversion profile and its wave propagation. A simple coarse-grained model is found to describe remarkably well the planar frontal logarithmic kinetics, capturing the effects of UV light exposure time (or dose) and temperature, as well as the front position. Furthermore, a unified mathematical expression for patterning, which is demonstrated in the predictive FPP fabrication of representative radical photopolymerizing networks, is proposed.

In defined conditions, surface instabilities are introduced in FPP and interfere with wave planarity, resulting in the formation of ‘minimal’ surfaces with complex 3D geometries. Building on this understanding on the propagation of wavefronts of network formation during photopolymerization, we demonstrate the design and fabrication of 3D patterned polymer materials with tunable shapes with optical and surface functionality.

Molecularly designed functional nanomaterials for energy and sustainability

Qilei Song^{ab}, S Cao^c, S Jiang^d, MF Jimenez Solomon^a, PS Fennell^a, AG Livingston^a, AI Cooper^d, AK Cheetham^c, E Sivaniah^{bf} 15:30–15:50

q.song@imperial.ac.uk

Sustainable energy supply and cleaner environment are key global challenges in the 21st century. Breakthrough technologies and step-change materials are desirable for natural gas production and conversion (The 21st century is the age of gas), renewable energy production and storage, CO₂ capture from fossil fuel combustion, and water purification and desalination. Novel functional nanomaterials hold great promises for solving these global challenges. Here I will briefly present our recent research on a range of functional nanomaterials with chemical structures defined on a molecular level, such as layered double hydroxides (LDHs), metal-organic frameworks (MOFs), polymers of intrinsic microporosity (PIMs), and molecular crystals such as porous organic cages (POCs). I will show our findings on understanding their structures and properties, and nano-scale fabrication of these materials towards applications in energy and environmental processes, such as nanostructured metal oxides for combustion and CO₂ capture, and high-performance sorbents and polymeric membranes for more efficient gas separations and water desalination. I will also highlight the broad potential of these functional nanomaterials and their derivatives including nanostructured carbon materials and composites, for high-performance electrodes and membranes in batteries and electrochemical devices for energy conversion and storage applications, which are new research programmes I am pursuing with the support of JRF fellowship and the department at Imperial College.

References:

1. Q. Song, W. Liu, C. D. Bohn, R. N. Harper, E. Sivaniah, S. A. Scott and J. S. Dennis. *Energy & Environmental Science*, 2013, 6, 288-298.
2. Q. Song, S.K. Nataraj, M. V. Roussenova, J. C. Tan, D. J. Hughes, W. Li, P. Bourgoïn, M. A. Alam, A. K. Cheetham, S. A. Al-Muhtaseb and E. Sivaniah. , *Energy & Environmental Science* 2012, 5, 8359–8369.
3. Q. Song, S. Cao, P. Zavala-Rivera, L.P. Lu, W. Li, Y. Ji, S.A. Al-Muhtaseb, A.K. Cheetham, E. Sivaniah, *Nature Communications*. 2013, 4, 1918.
4. Q. Song, S. Cao, R.H. Pritchard, B. Ghalei, S.A. Al-Muhtaseb, E.M. Terentjev, A.K. Cheetham, E. Sivaniah, *Nature Communications*. 2014, 5, 4813.
5. DHN Perera, Q Song, H Qiblawey, E Sivaniah. *Journal of Membrane Science*. 2015, 487, 74-82
6. Q. Song, S. Cao, R.H. Pritchard, E.M. Terentjev, A.K. Cheetham, and E. Sivaniah, 2015 (In submission).
7. Q. Song, S. Jiang, T. Hasell, M. Liu, A.K. Cheetham, E. Sivaniah, and A.I. Cooper, 2015, (In submission).

^aDepartment of Chemical Engineering, Imperial College London, London SW7 2AZ, UK; ^bCavendish Laboratory, Department of Physics, University of Cambridge, Cambridge, UK; ^cDepartment of Materials Science & Metallurgy, University of Cambridge, Cambridge, UK; ^dDepartment of Chemistry, University of Liverpool, Liverpool, UK; ^eDepartment of Chemical Engineering and Biotechnology, University of Cambridge, Cambridge, UK; ^fInstitute for Integrated Cell-Material Sciences (iCeMS), Kyoto University, Kyoto, Japan

Understanding cell rupture mechanisms in ultrasonication for bioprocessing applications

Angelo Pommella^a, NJ Brooks^b, JM Seddon^b, V Garbin^a 15:50–16:10

a.pommella@imperial.ac.uk

Ultrasonication is used in several bioprocessing applications to recover important products from cells, e.g. enzymes and proteins in the dairy and pharmaceutical industry, or lipids in algal biofuel production. During ultrasonication, large viscous stresses are generated due to cavitation and bubble dynamics. Despite its widespread application in industrial processes, so far only a few studies have investigated the mechanisms of cell rupture in the complex flows generated by ultrasonication. A better fundamental understanding of these mechanisms is required to exploit cell rupture in a more controlled fashion, and to minimise the energy cost of the process.

To study the mechanisms of cell rupture in a controlled fashion, in this project we used giant lipid vesicles as models for cells, to be able to precisely tune the mechanical properties of the lipid membrane and assess their effect on rupture conditions. The vesicles were exposed to the acoustic microstreaming flow generated by ultrasound-driven microbubbles, and their deformation and rupture was directly visualised by video microscopy. We identified conditions for selective breakup of vesicles based on the difference in membrane stretching elasticity, and investigated the effect of vesicle radius and excess area on the threshold for rupture. These results underpin the rational optimisation of ultrasonication processes for different cell types, and should enable new sorting mechanisms based on the difference in cell membrane composition and mechanical properties.

Reference

Pommella, A. et al. *Selective flow--induced vesicle rupture to sort by membrane mechanical properties*. *Sci. Rep.* 5, 13163 (2015)

^aDepartment of Chemical Engineering, Imperial College London, London SW7 2AZ, UK; ^bDepartment of Chemistry, Imperial College London, London SW7 2AZ, UK

Protein-polymer surfactant nanoconstructs for increased solubility and thermal stability in ionic liquids

Alex PS Brogan, JP Hallett

16:10–16:30

a.brogan@imperial.ac.uk

Ionic liquids, organic salts with melting temperatures below 100 °C, are becoming increasingly popular as solvents for many industrial. This is due to the multifarious, and highly tuneable, chemical and physical properties they possess, making them highly desirable for numerous applications. Biocatalysis has the potential to vastly improve the energy efficiency of many processes. This is due to the fact that enzymes can perform many industrially relevant reactions under significantly milder conditions than their chemical counterparts. However, the nonaqueous environments required are often destabilizing towards enzymes, and thus the window of usability can be limited. Therefore, there is now an impetus to develop new biotechnologies whereby proteins and enzymes can be stabilized in ionic liquids.

Here, we demonstrate that surface modification of proteins, through synthesis of protein-polymer surfactant nanoconstructs, yields a protein rich biofluid that exhibits high solubility in both hydrophilic and hydrophobic ionic liquids. Remarkably, we show that protein structure is highly conserved, and thermal stability of myoglobin is increased by 55 °C in the ionic liquid, as compared to aqueous solutions. As a result, this could become a platform technology for biocatalysis in anhydrous ionic liquids.

ATR-FTIR Spectroscopic imaging of dynamic processes

*Sir William
Wakeham
Award Lecture*

James A Kimber, SG Kazarian

16:30–16:55

james.kimber03@imperial.ac.uk

Attenuated total reflection Fourier transform infrared (ATR-FTIR) spectroscopic imaging is an emerging tool for the study of static and dynamic systems due to its chemical specificity, spatially resolved and label-free nature. The use of a focal plane array (FPA) detector allows for the acquisition of infrared spectra from different parts of a sample simultaneously, providing chemical snapshots of a system over time. ATR mode uses an inverted prism or crystal through which the infrared light interacts with the bottom surface layer of the sample. This enables the study of aqueous systems and samples under high temperatures and pressures, close to industrial conditions. Presented are two case studies, one studying pharmaceutical tablet dissolution and drug release in collaboration with AbbVie, and the other studying high-speed drying of latex films in collaboration with BASF.

In the first case, ibuprofen in salt or acid forms, with polymers Soluplus or copovidone, were combined using a hot melt extruder. The dissolution properties were assessed using ATR-FTIR imaging and UV/Vis detection. The marked differences in drug release properties were revealed from infrared spectra, indicating hydrogen bonding of the drug with the Soluplus but not with the copovidone, preventing water ingress for those formulations. The second case studied thin (20 μm) latex films drying under industrial conditions (high temperature air) in which high-speed ATR-FTIR imaging showed the distribution of water and polymer over time. Spectra were processed to produce drying curves in which two factors were identified and used to assess the performance of different latex formulations. The higher percentage of methyl methacrylate as a co-monomer and the use of n-Butylacrylate as the main monomer was shown to improve drying performance [2]. Both cases highlight the suitability ATR-FTIR imaging as a powerful approach to solve industrial problems.

[1] Pudlas, M., Kyremateng, S.O., Williams, L.A.M., Kimber, J.A., Lishaut, H., Kazarian, S.G., Woehrle, G.H., Analyzing the impact of different excipients on drug release behavior in hot-melt extrusion formulations using FTIR spectroscopic imaging, *European Journal of Pharmaceutical Sciences*, 2015, 67, 21-31

[2] Kimber, J.A., Gerst, M., Kazarian, S.G., Fast Drying and Film Formation of Latex Dispersions Studied with FTIR Spectroscopic Imaging, *Langmuir*, 2014, 30(45), 13588-13595

POSTER PRESENTATIONS

	Presenter	Poster title	Authors
1	Alessandra Vitale	X-ray reflectivity study of the surface oxidation of polydimethylsiloxane (PDMS) by plasma exposure and its impact on mechanical wrinkling	Manuela Nania, Fabrizia Foglia, Omar K. Matar, Joao T Cabral
2	Salman Masoudi Soltani	Industrial Separation of a Commercially-Emerging Refrigerant from Its Binary Mixture through a Bespoke Industrial Separation Process	Salman Masoudi Soltani, Paul S. Fennell
3	Qilei Song	Molecularly Designed Functional Nanomaterials for Energy and Sustainability	Qilei Song, S Cao, S Jiang, MF Jimenez Solomon, PS Fennell, AG Livingston, AI Cooper, AK Cheetham, E Sivaniah
4	Zhizhao Che	Bouncing and coalescence during oblique impact of droplets on flowing liquid films	Zhizhao Che, Omar K. Matar
5	Santanu Karan	Sub-10 nm polyamide nanofilms with ultrafast solvent transport for molecular separation	Santanu Karan, Z Jiang, AG Livingston
6	Lisa Kleiminger	3D Printing Functional Layers of Solid Oxide Fuel Cells and Electrolysers	L. Kleiminger, N.M. Farandos, A. Hankin and G.H. Kelsall
7	Vincentius Surya Kurnia Adi	Flexible Design for Photovoltaics/Fuel Cell/Wind Turbine (PVFCWT) Hybrid Power System	Vincentius Surya Kurnia Adi, Meng-Han Lin, Chuei-Tin Chang
8	Lyes Kahouadji	A Massive Parallel Solver for Direct Numerical Simulation of Three-Dimensional Multiphase Flows	L. Kahouadji, OK Matar, J Chergui, D Juric and S Sin
9	Sarah Fadda	A multi-scale strategy for understanding and improving recombinant protein glycosylation in CHO cells	Sarah Fadda and Cleo Kontoravdi
10	Agi Brandt-Talbot	Ionosolv Process: Recycling inexpensive ionic liquids for lignocellulose fractionation.	Agnieszka Brandt-Talbot, Tijs Lammens and Jason P. Hallett
11	Koen van Dam	Evaluating the financial incentives of smart charging schemes for electric vehicles drivers and aggregators	Elisabeth Mallet, Salvador Acha, Gonzalo Bustos Turu and Koen H. van Dam
12	Koen van Dam	Agent-based simulation as an urban design tool: Iterative evaluation of a smart city masterplan	Koen H. van Dam, Dietmar Koering, Gonzalo Bustos-Turu and Henry Jones, H.
13	Salvador Acha	Cost Effective Low Carbon Store analysis and Replication	Julien Box, Salvador Acha, Nilay Shah
14	Patrizia Marchetti	Tunable-porosity membranes for water treatment by discrete nanoparticle assembly	Patrizia Marchetti, Martin Mechelhoff, Andrew G. Livingston
15	Yolanda Sanchez-Vicente	Understanding the Thermophysical Properties of CO ₂ +H ₂ O/Brine Systems for Applications in Carbon Storage	S. Al-Ghafri, S. Cadogan, C. Calabrese, Y. F. Chow, J. Crawshaw, E. Efika, A. Georgiadis, R. Hoballah, X. Li, G. C. Maitland, E. May, M. McBride, C. Peng, Y. Sanchez-Vicente, M. S. P. Stevar J. P. M. Trusler