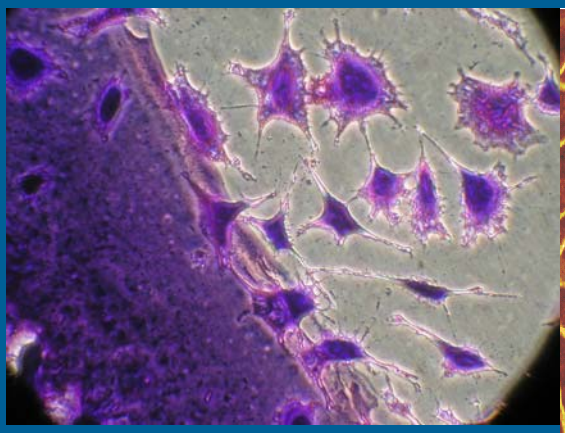
Centre for Self Organising
Molecular Systems

UNIVERSITY OF LEEDS

Annual Report
2006



CENTRE FOR
SELF ORGANISING MOLECULAR SYSTEMS
A UNIVERSITY OF LEEDS INTERDISCIPLINARY CENTRE

Centre for Self Organising Molecular Systems

Annual Report 2006

Contents

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Dr. John Colyer
Dr. Lars Jeuken

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SOMS Centre Secretary
Mrs. Virginia Antonie

Cover images: left - fibroblast cells attached to a piece of peptide gel, obtained by Dr Susan Felton; right - peptide nanotapes self-assembling at a solid-liquid interface, obtained by Dr Conor Whitehouse (aspect ratio altered for aesthetic purposes).

Foreward

The 2005/6 academic year began with a period of significant change for the SOMS Centre. On 1st October, I was appointed as Acting Director of the Centre, following the move of the previous Director, Prof. Ian Hamley, to a new position at Reading University over the Summer. I have the privilege of being the first "non-chemist" to occupy the role of Director the SOMS Centre, although, as a physicist currently working in an electronic engineering department, and with a history of research collaboration with the SOMS Centre since its inception in 1993, I believe that my 'interdisciplinary credentials' are pretty good! Nevertheless, even after serving on the SOMS Management Committee for several years, it has been a challenging and exhilarating experience to take on the leadership of the Centre.

All too often, University business, like all business, can become sidetracked by financial and political concerns. What I wanted to do first of all was to take SOMS back to its roots as an interdisciplinary research centre: to evaluate the current status of SOMS research, and to define a strategy for taking the research forward. I believe that this has been a fruitful process for all concerned: we have seen some excellent ideas emerge, and have developed an exciting and ambitious plan, both for expanding our long-standing research themes and for developing new themes (see page *) for details.

Interdisciplinary work is crucially dependent on communication, and another of my priorities was to rejuvenate our communication mechanisms both with our own members and with the wider research community in Leeds. Page * summarises the various SOMS events that were held during the year, along with plans for the 2006/7 events programme.

Part of the process of communication is restoring pride and confidence in the activities of a community. Our own research review, and our events programme, have shown us, and our peers, that there is much to be proud of in SOMS research, and that the long established track record and critical mass of expertise at Leeds in molecular self-organisation and self-assembly presents many opportunities for new research projects, collaboration and sponsorship.

Of course, SOMS activities are no longer limited to research. In 2005/6, the Centre welcomed its largest cohort of MSc students to date – 27 people studying either the Nanoscale Science and Technology or Nanoelectronics & Nanomechanics Masters programmes which are delivered in partnership with the University of Sheffield. Together with a total of 25 students distributed across the first 2 years of SOMS' Nanotechnology BSc programme, this makes for a substantial taught student community in the Centre. The Nanotechnology Masters activity is also expanding rapidly, with plans for at least 2 new programmes over the next 2 years, and the creation, in 2006, of an 'umbrella' brand – "Nanofolio" to describe the Leeds/Sheffield Nanotechnology Education activities.

All in all then, a busy year for SOMS, but one which has seen the Centre gain a new understanding of its purpose and direction, setting the scene for a successful 2007.

Robert W Kelsall
Leeds, October 2006

1. Research Strategy

For the past few years, research activity in the SOMS Centre has been focussed on three themes: self-assembling biomolecules, supported and suspended biomembranes, and discotic liquid crystals. During 2005/6, SOMS has been reviewing the research portfolio with the aims of defining the forward direction for the three existing themes, and identifying promising new themes for development.

For each of the existing themes, the forward direction can be categorised in terms of: (i) ongoing development of the basic materials & science; (ii) scale-up of the research, in terms of the range of materials involved and/or the production capacity, and (iii) development of applications.

Self-assembling biomolecules

Scale-up of the range of available materials will involve synthesis of artificial peptides to act as building blocks for the self-assembly of a range of nanostructures (collaboration with Schools of Chemistry & Colour Chemistry at Leeds). Scale-up of production volume will be pursued via non-food crops (with Faculty of Biological Sciences & Dept of Chemical Engineering at Leeds). Applications in templating, porous nanostructures, coatings, scaffolds, biomineralisation and antimicrobials will be developed (with Schools of Process, Environmental and Materials Engineering, Mechanical Engineering, and the Faculties of Dentistry and Biological Sciences).

Supported and suspended lipid membranes

The overall motivation of this research activity is for biosensor and biochip development. Further research will be carried out to improve the stability of the membranes, their support and tethering mechanisms, and to increase the range of surface modification options. Scale-up of the scope of the research will be achieved by systematically populating these artificial lipid membrane surfaces with biomembrane proteins, to create a complete range of model membrane systems, from the pure lipid bilayers to the fully populated biological membranes. Scale-up of volume is a longer term goal involving integration with arraying and delivery techniques and development of high-throughput systems. Applications will be investigated in the general areas of bio-interrogation, bio-sensing and bio-availability. Strategic collaborations are being developed with the membrane biology community at Leeds, within the Institute of Membrane and Sensor Biology and also the proposed Centre for Integrative Membrane Biology.

Discotic Liquid Crystals

The basic materials in this theme are now more mature than in the two other themes, with commercial applications in display coatings and as high pressure lubricants. Plans include scale-up of the scope of the work in two areas: (i) hybrid organic-inorganic structures and interfaces (with the School of Physics & Astronomy), and photoaddressable/ photochromic surfaces (with the Schools of Colour Chemistry and Physics & Astronomy).

New research themes

The three existing research themes will be complemented with one further materials-based theme, two themes based on scale-up of the basic science and concepts, and one new applications-oriented theme, as described below.

Molecular Self-assembly / Supramolecular chemistry
This materials-based theme concerns the synthesis of molecular 'building-blocks' which will self-assemble into larger molecular entities such as cages, synthetic zeolites and block co-polymers. The theme has synergies with the existing themes, but will add new dimensions via collaboration with researchers in Chemistry & Colour Chemistry. Work has already started on the development of a major interdisciplinary project in the application of molecular self-assembly to multi-dimensional nanopatterning. *For details contact Dr. Rob. Kelsall.*

Directed Assembly
The motivation of this theme is to exercise control over self-assembly/self-organisation processes and thereby achieve 'scale-up' by increasing the rate of assembly. Proposed projects include electric field directed assembly of vesicles, electric field directed transport of amphiphiles, along with the investigation of other electromagnetic and magnetostatic fields for direction of assembly. The theme will involve collaboration with the Schools of Process, Environmental & Materials Engineering, Mechanical Engineering, Food Science, and Colour Chemistry. *For details contact Dr. Andrew Nelson.*

Excitable biosystems assembly
The aim of the theme is to investigate assembly on a cellular, rather than a molecular level, and specifically, for SOMS, to understand how the principles of molecular self-assembly/organisation translate to the cellular level. As such, this theme also has 'scale-up' as its underlying idea, and is a natural complement to the Directed Assembly theme. This theme will comprise one facet of the extensive excitable systems biology consortium at Leeds, and will involve collaboration with the Faculty of Biological Sciences and with the School of Mathematics. *For details contact Dr. John Colyer*

Nanoparticle toxicity
This is an applications-oriented theme which will be based largely on the technology developed in the lipid membranes research theme. Whilst there are many aspects of nanoparticle toxicity which lie outside SOMS' range of expertise, it has become clear that the lipid membrane biosensors represent a powerful and uncommon tool for this application. The aims of this theme will be to encourage the development of membrane biosensors specifically for nanoparticle toxicity assessment, and also to identify and co-ordinate a university-wide consortium which, together, possesses the range of skills needed to address the problem overall. *For details contact Dr. Andrew Nelson.*

SOMS research currently involves 7 academic staff directly associated with the Centre, plus a further ~20 staff across the campus. The plans for new themes, and development of existing themes, will increase the level of participation to an estimated total of over 40 academic staff. A series of 1 or ½ day discussion meetings is being scheduled to launch the new themes, define strategic actions, and identify theme leaders.

2. Research reports

2.1. Self-assembling biomolecules *(theme leader, Dr. A. Aggeli)*

In the last year we have carried out research with the aims of: a) understanding the fundamental physical and chemical principles that drive beta-sheet peptide self-assembly and b) harnessing this insight into the fabrication of designed peptidic nanostructured materials and devices with a combination of desirable properties appropriate for nanotechnology, the chemical and the pharmaceutical industries.

Beta-sheet forming peptides can behave like chiral rod-like building blocks and, under the appropriate solution conditions, they self-assemble in one-dimension to give rise to a hierarchy of well-defined micron-long nanostructures such as tapes (single molecule thick), ribbons (two stacked tapes), fibrils (several ribbons stacked and twisted together) and fibres (two fibrils entwined edge-to-edge). In an attempt to start quantifying the relationship between peptide molecular properties and self-assembling behaviour, a range of complementary physicochemical techniques were employed including computer molecular modelling, infrared, circular dichroism UV and NMR spectroscopies and light scattering (*1*). Such studies have begun to reveal the dynamic behaviour of the self-assembled tapes, ribbons and fibrils as well as the effects of the molecular parameters on their formation and stabilisation (Fig. 1). At high enough concentration in solution (semi dilute regime), these polymers can form nematic fluids and gels, hydrogels and organogels. A unique property of such systems is that the self-assembling and material properties (gel versus fluid) can be controlled by external chemical or physical triggers. This can provide important processing opportunities for the chemical industry. To demonstrate this property a range of peptides were designed whose solutions were seen to switch from an isotropic Newtonian fluid to a nematic gel state by small pH changes or by mixing complementary peptide solutions.

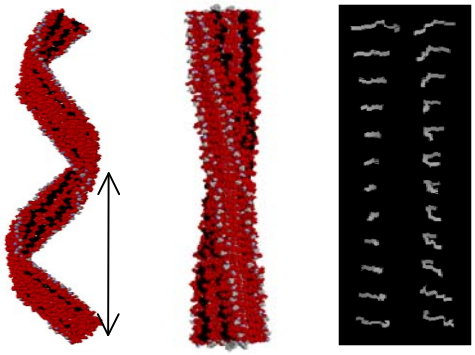

Fig. 1. Molecular models of peptide tapes and ribbons (*2*).

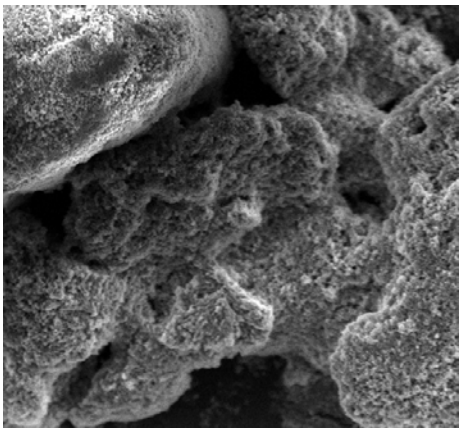

Fig. 2. SEM micrograph of hydroxyapatite crystals nucleated inside a peptide gel.

In collaboration with Prof. J. Kirkham and C Robinson (Dental School, Univ. Leeds), Ca^{+2}- binding peptide gels have been self-assembled *in situ* in teeth caries-like lesions and have been shown to increase enamel remineralisation which can lead to tooth repair (Fig. 2). This property has been ascribed partly to the ability of the peptide fibrils to template hydroxyapatite crystals mimicking the natural process of biomineralisation, and may have wider implications for usage of self-assembling materials in bone tissue engineering (*3*). In another collaboration with Profs J. Fisher (Dept of Mechanical Engineering and Institute of Medical and

Biological Engineering, Univ. Leeds) and E.Ingham (Microbiology & IMBE, Univ. Leeds) peptide hydrogels in physiological solution conditions have been developed and evaluated as injectable biolubricants in osteoarthritic joints (*4*).

Self-assembly of beta-sheet tape forming peptides has been studied not only in bulk solution as described above, but also in two other environments, namely on solid substrates and in lipid bilayers. Tapes are biaxial structures (compared to eg uniaxial rod-like structures), thus they are expected to have unique surface properties. Indeed peptides in their monomeric state in solution have been seen to self-assemble directly into tapes sitting flat on a solid substrate, such as mica or graphite (Fig. 3). The peptides are designed such that the lower side of the tape interacts favourably with the solid surface, whilst its upper side interacts favourably with the solvent. The tapes form on the surface until the substrate gets covered with one-molecule thick coating of tapes. The self-assembly of peptide tapes in the presence of the two-dimensional constraints of a lipid bilayer or a lipid monolayer (*6*) has also been studied. The investigations carried out so far indicate that amphiphilic peptide tapes bend around to form a closed beta-barrel-like structure, reminiscent of porins, which transverses the lipid bilayer and acts as an ion-channel. These structures are stabilised due to the need to satisfy the complementary hydrogen bonding groups of the peptide backbone of the first and the last beta-strand in the tape in the hydrophobic interior of the lipid membrane.

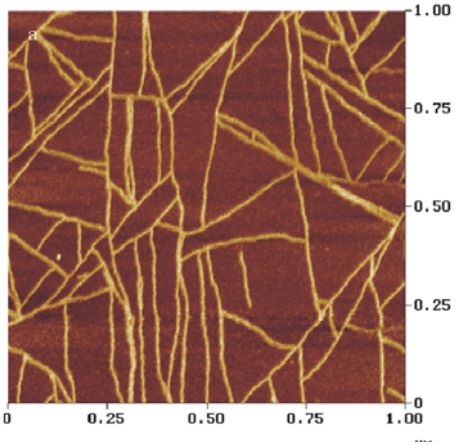

Fig. 3. Peptide tapes forming on a mica surface from their monomeric state in solution (*5*).

The results were published in six peer-reviewed publications and a book chapter and presented in a number of national and international conferences, e.g. in Australia and Greece and at several invited industrial seminars. The projects are currently run by ten PhD students and two postdoctoral researchers, funded by the European Union, EPSRC, the Royal Society, the Dutch Polymer Institute and the chemical and pharmaceutical industry, with a total of more than £2m of external funding at present. The plans for the next year include :

- continue establishing a quantitative relationship between peptide molecular properties and their self-assembling properties, and derive magnitudes of energetic parameters that drive self-assembly in solution and at interfaces (solid substrates, as well as in lipid bilayers);
- explore the possible usefulness of these systems in a wide range of applications, such as in nanotechnology, chemical industry, biology and medicine.

List of publications 2005-2006

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2. Davies RPW, Aggeli A, Beevers AJ, Boden N, Carrick LM, Fishwick CWG, McLeish TCB, Nyrkova I, Semenov AN, Self-assembling beta-sheet tape forming peptides, *Supramolecular Chemistry*, vol. 18, 435-443, 2006

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4. Bell CJ, Carrick LM, Katta J, Jin ZM, Ingham E, Aggeli A, Boden N, Waigh TA, Fisher J , Self-assembling peptides as injectable lubricants for osteoarthritis, *Journal of Biomedical Materials Research Part A*, vol. 78A, 236-246, 2006

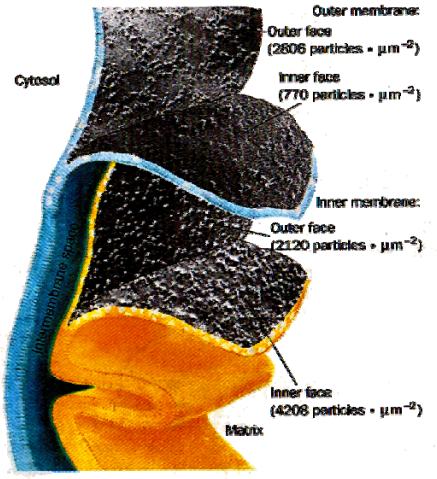
5. Whitehouse, C, Fang, J, Aggeli, A, Bell, M, Brydson, R, Fishwick, C, Henderson, J, Knobler, CM, Owens, RW, Thomson, NH, Smith, DA & Boden, N, Adsorption and self-assembly of peptides on mica substrates, *Angewandte Chemie Int. Ed.*, vol. 44, 1965-1968 2005.

6. Protopapa, E., Aggeli, A., Boden, N., Knowles P F, Salay, L. C. and Nelson, A., Interaction of self-assembling beta-sheet peptides with phospholipid monolayers, *Medical Engineering & Physic*s, vol 28, 944-955, 2006

7. Aggeli, A, Boden, N, Carrick, L, McLeish, TCB, Nyrkova, IA, & Semenov, AN, Self-assembling peptide gels in *Molecular Gels*, editors P.Terech & R.G.Weiss, Kluwer Academic Press, 2005.

2.2. Supported & Suspended Biomembranes *(theme leader, Dr. L. Jeuken)*

Biological membranes have a wide variety of essential tasks, ranging from cellular nutrition and drug uptake to neurotransmission. The membranes of cells are selective barriers and drug and/or toxins will have no effect if they cannot pass them. But the opening of channels in a membrane serves a much wider task than just the uptake of chemicals by cell. Also signals need to pass the membrane before they can affect the cell and signal transduction is regulated by the membrane.



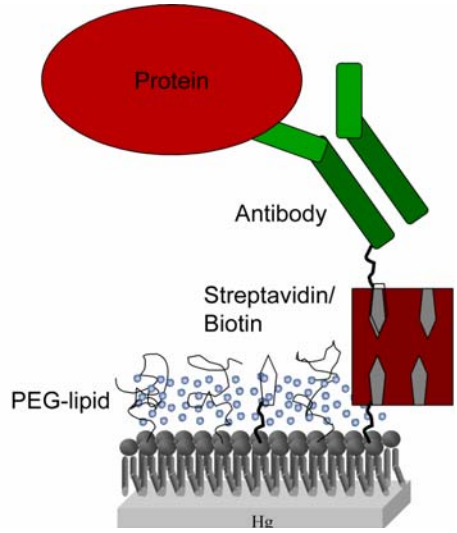
Freeze-fracture and freeze-etch electron micrographs of the inner and outer mitochondrial membranes. Picture taken from Voet, Voet and Pratt in *Biochemistry*

At the SOMS centre, biological membranes form an important research theme which focuses on the coupling of biomembranes and solid surfaces (electrodes). This hybrid bio-electronic technology permits molecular signals to be converted real-time into electronic information and allow the translation of biological signals in clear and concise electronic signals or the detailed mechanistic study of biological processes like metabolism. Over the last one to two years we have passed several milestones in:

1) Sensitive and protein/peptide specific sensor applications.
2) Understanding the effects of electric field on lipid structure and insertion of pharmaceutical compounds and peptides in a lipid layer.
3) Use of bacterial biological membranes in the fabrication of hybrid membrane-electrode technology.
4) Formation of complicated biological architectures like cell walls and cytoskeleton scaffolds on the membrane surface to extend our biomimicking applications.
5) Electron transfer from the surface into membrane-bound redox-active enzymes, allowing the detailed mechanistic study of these enzymes.
6) Use of membrane-protein engineering for the construction of tailor-made sensors.

Sensitive and protein/peptide specific sensor applications
(Dr. P.A. Millner and Dr. A. Nelson)

Phospholipid monolayers on mercury form a unique system of 'supported model membranes' which are ideal for sensitive measurement of a wide variety of molecular interactions and also the behaviour of phospholipid layers in an electric field (*1*). These latter studies provide a fundamental understanding of the physical mechanisms which underlie electroporation in bilayers and cell membranes. The membrane layers are defect-free, self-sealing and impermeable to ions. Any interaction between the supported membranes and soluble compounds result in an immediate signal obtained by impedance spectroscopy.

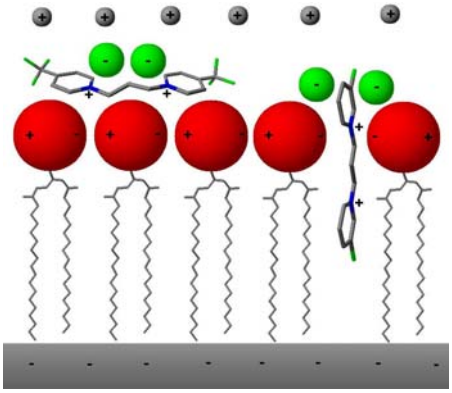


Schematic representation of the biosensor technology developed at SOMS

A long-standing problem in any sensitive bio-sensor application is the a-specific binding of molecules often present in large excess to the target molecule. In order to detect specific protein binding, the group of Dr. A. Nelson in collaboration with Dr P. A. Millner has developed a system that suppresses or even abolishes a-specific binding and a test system that detects haemoglobin via a antibody interaction has been prepared(*2*).

Effects of electric field (Dr. A. Aggeli and Dr. A. Nelson)

The extreme sensitivity of the phospholipid coated mercury surface also has pharmaceutical application and lipid interactions have been characterised with: (a) bispyridinium compounds(*3*), used as treatment against nerve agents, (b) the human anti-microbial peptide LL-37(*4*) and self assembling β sheet peptides in collaboration with Dr A. Aggeli (*5*) and (c) *ex situ* reconstructed sea surface microlayers.(*6*) The fluid nature of mercury also allows for detailed studies of alkanethiol supported layers (*7*) and of interactions in other adsorbed films(*8*).

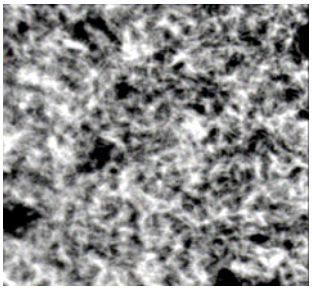


Schematic representation of the interaction between bispyridinium and the phospholipid membrane as determined by the group of A. Nelson. Green are iodide anions and grey are potassium ions.

Model membranes prepared from bacterial membranes
(Dr. L.J.C. Jeuken, Prof. R.J. Bushby and Prof. S.D. Evans)

Hybrid membrane-electrode devices are commonly prepared from purified phospholipids only. Some success by the groups of Dr. Jeuken and Prof. Evans has been obtained by incorporating membrane proteins in these devices(*8, 9*). However, this is a technologically complicated process with variable results. At SOMS we have developed new methods in which the whole bacterial membrane, which consist for up to 60% of protein, is bound to a surface. This novel type of system is very powerful in studying complex processes such as cell wall formation or electron transfer in the metabolic electron transport chain(*10, 11*).

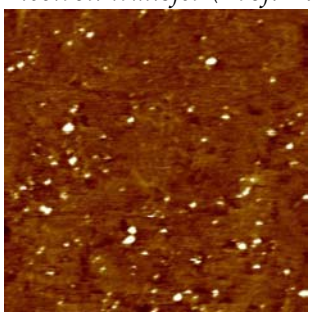
Cell walls and cytoskeletons (Prof. R.J. Bushby, Dr. J. Colyer and Prof. S.D. Evans)



Fluorescent actin filaments bound to a hybrid membrane electrode surface

Cell membranes in biology are complicated structures which extend beyond the central lipid bilayer with membrane proteins. In order to fabricate accurate membrane biomimics, bacterial cell walls and actin 'scaffold' have been constructed on top of our hybrid membrane-electrode systems. Bacterial cell walls have been formed on bacterial membrane surfaces by supplying the chemical building blocks of a cell wall and using the natural enzymes in the bacterial membrane to form the chemical bonds needed to form the cell wall polymer(*10*). This system will have direct application in the study of cell wall formation and inhibition thereof by (potential) anti-biotic reagents. Actin scaffolds have been formed by incorporating a small membrane protein, ponticulin, in the hybrid membrane-electrode system which function in biology is to nucleate actin polymerisation and to serve as an anchor point of the actin polymer.

Electron transfer (Prof. R.J. Bushby, Prof. S.D. Evans and Dr. L.J.C. Jeuken,)

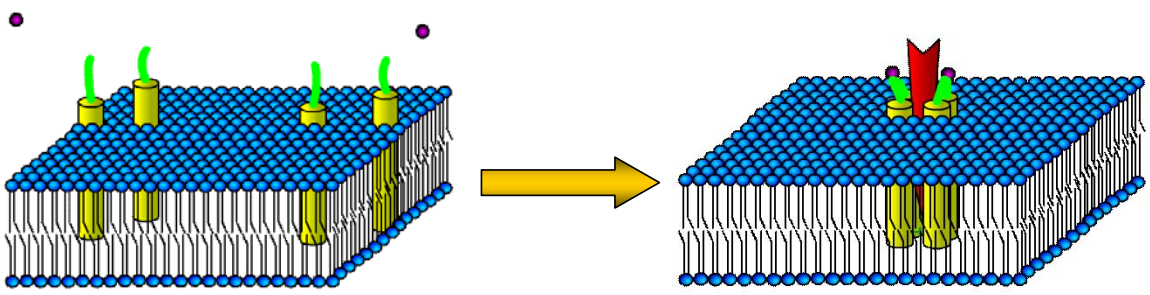


AFM image of ubiqionol oxidase incorporated into a hybrid membrane electrode surface

Electron and charge transport in and across the membrane is an important aspect of membrane biology. SOMS has used the hybrid membrane-electrode platform to study two membrane-bound redox-active membrane proteins, a succinate-menaquinone oxidoreductase (*11*) and an ubiquinol oxidase (*9*). Electrons were efficiently transferred between the electrode surface and the enzymes via the naturally occurring quinone pool, which in nature is also used to pass electrons (and protons) between enzymes and across the membrane.

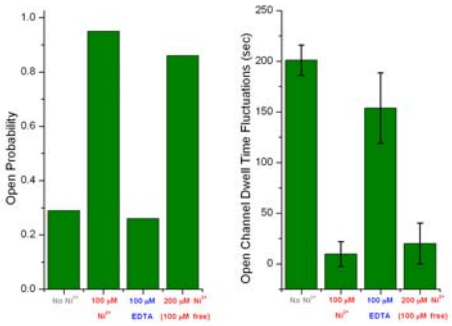
Tailor-made ion-channels (Prof. S.D. Evans and Dr. J. Colyer)

Ion channels are biological way of signal amplification. After triggering an ion channel to open by for instance adding a ligand, many ions will flow through the lipid membrane, amplifying the signal resulting from a single molecule. In order to apply this feature in tailor-made ion channels for biosensors, the group of Dr. J. Colyer has designed several peptides based on the M2 protein.(*12*) The M2 protein is a proton-selective ion channel



A schematic representation of the tailor-made biosensor based on M2 protein.

protein, integral in the cell membrane of the influenza A virus. The channel is a homotetramer (consists of four identical M2 units) and only 'opens' when all four units are properly assembled. By selectively changing the amino acid sequence of M2, the proton-selectivity was released and by adding a histidine to the end of the sequence, a tailor-made trigger was introduced. When metals are added to the ion-channel, they bind multiple histidines, increasing the probability four units come together and open a channel.



Histograms showing the differences in open probability (left) and open channel dwell time fluctuations (right) before and after the sequential addition and removal of Ni^{2+} ions

International collaborations and visitors

Dr Blazenka Gasparovic from the Rudjer Boskovic Institute, Croatia visited three times in the period as part of a Royal Society project and one publication (6) ensued. Lovisa Ringstad from Uppsala University, Sweden worked also in the group in May on synthetic antimicrobial biomembrane activity. Dr Britta Sethson from Umea University, Sweden visited in October as part of a EU FW6 programme substituting animal testing of pharmaceuticals with surface chemical methods.

Summary and future planning

These results were published in twelve peer-reviewed publications presented in a number of national and international conferences. The projects are currently continued by three PhD students and six postdoctoral researchers, funded by the EPSRC, BBSRC, Royal Society, EPSON, MoD-DSTL, RSC, Leeds Nanomanufacturing Institute, the Health & Safety Laboratory and the European Union. The plans for the next year include:

- (continue to) prepare micro to nanoscale substrates to serve as array platforms for the supported bilayers. This includes devices that contain small reservoirs which will enables us to measure transmembrane charge transport more accurately.
- use tethered vesicles filled with pH sensitive dyes to study proton-pumping enzymes using a combination of electrochemistry and fluorescence spectroscopy.
- continue the work on actin and cell-walls and perform microscopic and spectroscopic characterisation to increase our understanding of these platforms.
- continue using phospholipid coated electrodes to screen the biomembrane activity of self assembling β sheet peptides, synthetic anti microbial peptides and alzheimer peptides.
- transforming the phospholipid coated mercury system to a robust sensing device. This involves using thin film mercury coated iridium electrodes arranged in a microfabricated array (collaborative work with Dr. P. Steenson).

List of publications

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2. Weiss, S., Millner, P., and Nelson, A. (2005) *Electrochim. Acta 50*, 4248-4256.

3. Merrifield, J., Tattersall, J. E. H., Bird, M., and Nelson, A. (2006) *Electroanalysis In press*.

4. Neville, F., Gidalevitz, D., Kale, G., and Nelson, A. (2006) *Bioelectrochem. In press*.

5. Protopapa, E., Aggeli, A., Boden, N., Knowles, P. F., Salay, L. C. and Nelson, A., (2006) *Medical Engineering and Physics* 28, 944-955

6. Frka, S., Nelson, A., and Kozarac, Z. (2006) *Int. J. Environ. Anal. Chem. 86*, 325-335.

7. Cohen-Atiya, M., Nelson, A., and Mandler, D. (2006) *J. Electroanal. Chem. 593*, 227-240.

8. Gasparovic, B., Risovic, D., Cosovic, B., and Nelson, A. (2006) *Electrochim. Acta In press*.

9. Johnson, B. R. G., Bushby, R. J., Colyer, J., and Evans, S. D. (2006) *Biophys. J. 90*, L21-L23.

10. Jeuken, L. J. C., Connell, S. D., Henderson, P. J. F., Gennis, R. B., Evans, S. D., and Bushby, R. J. (2006) *J. Am. Chem. Soc. 128*, 1711-1716.

11. Spencelayh, M. J., Cheng, Y. L., Bushby, R. J., Bugg, T. D. H., Li, J. J., Henderson, P. L. F., O'Reilly, J., and Evans, S. D. (2006) *Angew. Chem.-Int. Edit. 45*, 2111-2116.

12. Jeuken, L. J. C., Connell, S. D., Nurnabi, M., O'Reilly, J., Henderson, P. J. F., Evans, S. D., and Bushby, R. J. (2005) *Langmuir 21*, 1481-1488.

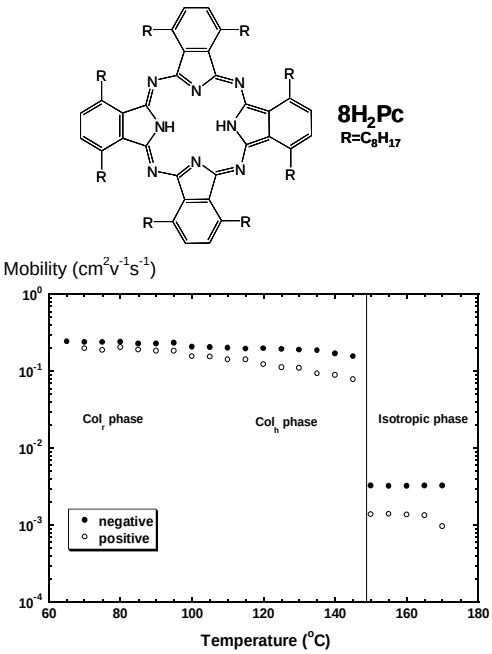
13. Bacchus, P. S. (Thesis 2006) *Ion Channel Reporter Technology*, Faculty of Biological Sciences, University of Leeds, Leeds.

2.3 Discotic Liquid Crystals *(theme leader, Prof. R. J Bushby)*

Discotic liquid crystal have only been known for about thirty years and applications may be modest in comparison to the much longer established calamitic liquid crystals. Sales of calamitic liquid crystal displays run at ca 35 billion US$ pa) but sales of discotics are growing. Their use as optical compensating films (to improve the angle of view of displays) is now well established and this year Fuji launched a new range of specialist discotic liquid crystal-based lubricants. Apparently their performance at high pressures is exceptional. Our interest in them is as self-organising/self-repairing organic semiconductors. It is a field of research which we began at Leeds and which is continuing to grow word-wide. We are interested in all aspects of the problem – synthesis of the liquid crystals – characterisation of their conductive properties– the theory of conduction.

Highlights of our recently published and current work are:

1. The discovery of the best (highest mobility) liquid crystal so far: the phthalocyanine derivative shown in the figure. It not only has exceptionally high mobility but is a carrier for both holes (positive charges) and electrons (negative charges). Organic conductors such as this are of increasing importance commercially. They cannot rival silicon for some 'high-end' applications but in other areas (for example the printing of electronic tags which will eventually replace bar codes) they win out over conventional materials because they are so much cheaper to process.



High conductivity phthalocyanine derivative and temperature dependence of its electron and hole mobilities.

2. Modelling work which suggests a possible way to understand charge migration in high-mobility discotics. For these and other organic conductors with mobilities of about one neither of the established models of conduction (band or hopping) is really satisfactory.

3. Extensions to our ferric chloride/methanol method of synthesising triphenylene-based discotics. This is the route use for the synthesis of all commercial discotic liquid crystals and – on the basis that our first paper on this is one of their most cited papers ever - we have been invited to contribute a commentary on it to a special anniversary issue of the journal *Liquid Crystals* which will be published at the end of the year

The discotic liquid crystal group in SOMS has reduced in size recently, due to staff moves and retirements, but currently includes five PhD students with industrial support from both

Merck and ICI. Thirteen papers were published in 2005 and 2006 to date, with many more in progress.

Future plans for this research theme involve diversification, building on the knowledge gained of discotic liquid crystals:

i) to investigate the physical and chemical properties of hybrid organic-inorganic structures and interfaces (including hybrid discotic liquid crystal – inorganic structures, but also considering other organic molecules),

ii) to develop photoaddressable and photochromic surfaces by synthesis of optically-active discotic liquid crystal derivatives.

List of selected publications 2005/6

A McNeill, R.J. Bushby, S.D.Evans, Q. Liu, and B. Movaghar, 'Discotic liquid crystals' in '3D nanoelectronic Computer Architecture and Implementation' ed. D. Crawley, k. Nikolic and M. Forshaw, IoP Publishing, 2005, Chapter 9, pp 203-223.

L. J. Lever, R.W. Kelsall, and R.J. Bushby, 'Band transport model for discotic liquid crystals *Physical Review B*, 2005, **72**, 035130.

L. J. Lever, R J Bushby and R W Kelsall, "A Band Transport Model for Highly Ordered Discotic Mesophases" *Journal of Computational Electronics* **4** 101-4 (2005)

R.J. Bushby, I.W. Hamley, Q. Liu, O.R. Lozman and J.E. Lydon, 'Self-assembled columns of fullerene' *Journal of Materials Chemistry*, 2005, 15, 4429..

H. Iino, Y Takayashi, J.Hanna and R.J.Bushby, 'Fast Ambipolar Carrier Transport and East Homeotropic Alignment in a Metal-Free Phthalocyanine Derivative', *Japanese Journal of Applied Physics*, 2005, **44**, L1310-L1312.

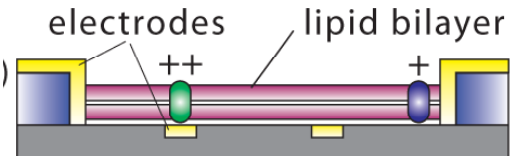
H. Iino, Y Takayashi, J.Hanna, R.J.Bushby and D. Haarer, 'High electron mobility of 0.1 $cm^2 V^{-1}s^{-1}$ in the highly ordered columnar phase of hexahexylthiotriphenylene' *Applied Physics Letters*, 2005, **87**, 192105.

H. Iino, J. Hanna, D. Haarer and R.J. Bushby, 'Fast electronic transport in discotic columnar phases of triphenylene derivatives' *Japanese Journal of Applied Physics Part1*, 2006, **45**, 430-433.

H. Iino, J. Hanna, R.J. Bushby and B.J.Whittaker, Conductivity in a discotic liquid crystal with a strong lateral dipole moment, *Journal of Applied Physics*, 2006, 110, 043716.

2.4 Programmable Dynamic Surfaces (*SOMS contact: Prof. R J Bushby)*

The majority of, if not all, surfaces employed for device fabrication and sensing applications are solid – they present an immobile hard support to which organic and inorganic materials can be attached, and patterned. Generally the surface itself plays a passive role, and following deposition there is little one can do to change the location of assembled elements. We will exploit the in-plane fluidity of phospholipid bilayers to create novel dynamic surfaces. Such surfaces could form a programmable template for the delivery and deposition of inorganic or biological nanoscale elements, or could create arrays with biological specificity. While it is premature to predict the ultimate application of such surfaces, there will be significant, and useful, milestones – e.g. in the controlled separation, and 2D-crystallization of membrane proteins. Lipid bilayer membranes provide the dynamic 'fluid' phase in which lipid molecules and proteins are free to diffuse (or if charged, driven by an external electric field) within the bilayer plane. We will develop the technology to direct charged membrane proteins through patterned geometries of fluid lipid bilayers by electric fields. This will allow the proteins to be separated by their charge/mass ratio or directed to specific locations for further exploitation.



Manipulation of a fluid lipid surface

This research is supported by a RCUK Basic Technology grant on "Biofunctionalised surfaces", total value ~£2.5M, and involves collaboration between SOMS (R J Bushby and S D Evans), the School of Physics & Astronomy (S D Evans), the School of Electronic & Electrical Engineering (A G Davies) and the Faculty of Biological Sciences (P Stockley).

3. Education and training

The SOMS Centre currently runs two interrelated Nanotechnology Masters programmes – the MSc in Nanoscale Science and Technology, and the MSc Nanoelectronics and Nanomechanics. Both programmes are managed and delivered in partnership with Sheffield University: a pioneering arrangement which has proved so successful that it has established an international reputation for innovation and excellence in nanotechnology education.

The original Masters programme, Nanoscale Science and Technology, is now in its 5th year of delivery, and the combined MSC cohort in 2005/6 was a record of 27 students. The MSc programmes were originally funded by EPSRC via a Masters Training Package grant, and are currently supported by Leeds' EPSRC Collaborative Training Account. The future strategy for the Masters portfolio involves, on the one hand, expansion of the portfolio to widen the market base, and on the other hand, development of alternative income streams in order to move towards financial self-sufficiency.

Expansion will involve a 3rd inter-related MSc in Nanomaterials for Nanoengineering, scheduled for entry from Sep 2006, a 4th MSc in Bionanotechnology (scheduled for Sep. 2007 launch), and a further MSc in Nanomanufacturing (provisionally scheduled for Sep. 2008). The Bionanotechnology MSc represents a long-standing aim to open our provision to life-science graduates, and has already been supported by a new academic staff appointment at Sheffield. The Nanomanufacturing MSc will be developed in partnership with the Leeds Nanomanufacturing Institute (NMI), and will be aimed, primarily, at the industrial market. The potential market for this MSc will be assessed by running a series of precursor industrial short courses, which will be organised by the NMI.

Development of alternative income streams will be achieved, in part, by intensifying recruitment in strategically significant international markets, but also by the development of a sustainable short course / workshop programme. The MSc programmes were originally designed with a view to adaptation for short course delivery, and so several modules are directly amenable to this development. The first such course, a 1 week course on Nanocharacterisation, will be delivered in October 2006. International recruitment was boosted by the launch of an international scholarships scheme. These scholarships are valued at £1500 per year, and are awarded on a competitive basis to candidates applying from outside the European Union.

The substantial growth in the number of programmes and related training activities offered created a need for a concise and memorable 'descriptor' for the activity. Therefore, in 2006, "Nanofolio" was launched. The name is a shorthand for "The universities of Leeds and Sheffield Nanotechnology Education Portfolio": Nanofolio encompasses all our present and planned activities in this sphere which are conducted jointly by Leeds and Sheffield. The Nanotechnology MSc website has been fully rebuilt, expanded, and relaunched as the Nanofolio website (www.nanofolio.org), and a distinctive Nanofolio logo has been created (see adjacent).

nanofolio
The Universities of Leeds and Sheffield
Nanotechnology Education Portfolio

In addition to the Nanofolio courses, SOMS also runs a 3 year BSc programme in Nanotechnology. This programme is highly multidisciplinary, involving collaboration with six departments at Leeds, and provides a broad-based physical and life sciences education in parallel with practical experience in state-of-art nanotechnology techniques. An additional feature of the programme is its coverage of the social, environmental and ethical issues associated with the development of new technologies at the Nanoscale. The SOMS Nanotechnology BSc is currently the only integrated nanotechnology undergraduate programme in the UK, although several universities have aspirations to develop similar programmes. Leeds, through SOMS, is therefore well ahead of the competition in this respect, and we must consolidate our leading position as undergraduate demand for nanotechnology education begins to grow. The programme recruited up to its quota of 15 students in 2005.

Overall, the aim of the SOMS teaching portfolio is to deliver programmes which support the University of Leeds' strategic ambition of world-class teaching in terms of innovation, research-informed education and high quality student experience.

4. **SOMS Events 2005/6**

Nov. 25th 2005 — *SOMS Poster Afternoon*
SOMS researchers presented posters of their recent work at a new event open to all Leeds personnel. A good networking opportunity in an informal environment. Organised by SOMS PhD student, Lucy Holt.

January 16th 2006 — *Discotic liquid crystals ½ day research strategy meeting*

January 19th 2006 — *Biomembranes ½ day research strategy meeting*

May 10th 2006 — *Nanotoxicity 1-day workshop (co-organised with Leeds NMI)*
A major exploratory workshop with the aim of bringing together Leeds researchers with expertise which could contribute to the emerging field of nanoparticle toxicity. See page * for full report.

May 17th 2006 — *Molecular Assembly ½ day meeting*
The initial meeting of this new research theme area, with presentations of individual research activities, and discussions on collaborations and research proposal developments. The main outcome of this meeting was a decision to develop a major project on molecular self-assembly for 3-dimensional nanopatterning.

June 20th 2006 — *Nanotechnology Masters Project Presentation Day*
This annual event is one of the highlights of the Nanotechnology MSc calendar. All our MSc students give presentations to an audience comprising Leeds and Sheffield academic staff and students, and members of the MSc Industrial Advisory Board. Students, staff and industrialists also meet informally over lunch.

June 26th 2006 — *SOMS Annual General Meeting*
Report on the year's activities and presentation of the newly developed SOMS research strategy to all SOMS members.

June 29th 2006 — *Nanotechnology teachers open day*
A new event for secondary school science teachers combining laboratory tours, demonstrations and informal discussions, along with information about the BSc Nanotechnology programme.

SOMS/NMI 1-day workshop on Nanoparticle Toxicity
May 10th 2006

Aims: To determine the overall capability at Leeds for research on the scientific aspects of nanoparticle toxicity - including sensing & interrogation of chemical and biological interactions, modelling and characterisation, and the impact on human health and on the environment – and hence optimise Leeds' potential for engagement with government & industrial sponsors in this area.

Presentations:

Overview of nanoparticle toxicity issues:	Dr. Sean Kelly, Leeds Nanomanufacturing Institute
Lipid membrane sensors:	Dr Andrew Nelson, SOMS
Invertebrate toxicology:	Prof. Elwyn Isaac, Faculty of Biological Sciences
Characterisation of Nanoparticles:	Dr. Andrew Brown, Inst. of Materials Research
Modelling issues:	Dr. Robert W Kelsall, SOMS
Environmental effects:	Dr. Mike Routledge, Molecular Epidemiology

Three breakout discussion groups were convened, with the sub-themes "*Membranes & sensors", "Modelling & characterisation" and " Human health & environmental issues".* Relevant strengths at Leeds were identified in the following areas:

- membrane biology, biochemistry and biophysics, and related devices
- cellular biology including cytotoxicity and immunology
- tissue and organ research
- whole organism research (vertebrates and invertebrates), including regulatory toxicology
- epidemiology (eg., cancer, diabetes, cardiovascular)
- nanoparticle preparation
- electron microscopy and associated elemental analysis

Weaknesses identified included the lack of a central toxicology institute, the lack of detailed computational modelling of interactions between nanoparticles and membranes or cells, the current absence of communication between the diverse groups mentioned above

Opportunities were identified:

- in capitalising on the strengths in membrane science and particle preparation/characterisation by developing membrane screening methodologies for a wide range of different Nanoparticles
- in exploring the extent of the overall capability at Leeds for developing a hierarchy of screening approaches, from the membrane level to the organism level

It was concluded that the Leeds strengths were complementary to the traditional toxicology routes, and were valuable for developing understanding of the underlying science. The range of substances which may be broadly termed as nanoparticles is so diverse that extensive testing of different particles, and therefore detailed structural and chemical characterisation of particles, is essential.

The Leeds Nanoparticle Toxicity community will continue to develop. Expressions of interest from both internal and external collaborators are most welcome. Please contact the SOMS Centre Director.

SOMS Seminar series
Fridays at 1pm.
2005/6 speakers:

Dr Toby Jenkins (Dept. of Chemistry, University of Bath), *Molecular structuring of surfaces for biosensing*

Dr Alexei Nabok (Dept. of Physics, Sheffield Hallam University), *Registration of toxins with total internal reflection ellipsometry*

Dr Christoph Walti (School of Electronic & Electrical Eng., Leeds), *Engineering at the nanoscale by self-assembly*

Dr Jim Burger (Umea University, Sweden), *Multivariate Hyperspectral Image Analysis*

Dr Richard Clayton, (University of Sheffield), *Continuous and discrete models of propagation in cardiac tissue*

Prof. Richard Templer (Imperial College), *Evidence that drugs eat their way across cell membranes*

Dr. Jan Philip Judson (Lhasa Ltd, Leeds), *Trying to Think Like a Chemist - The Lhasa Project in Computing*

Ibon Odriozola (SOMS Centre, Leeds), *Synthetic helical molecular systems. Design, synthesis and coiling/uncoiling properties*

Dr. John Sanderson (University of Durham), *Self-Assembling Systems for Studying Protein-Lipid Interactions*

Dr. Sarah Harris (School of Physics & Astronomy, Leeds), *Molecular Dynamics Simulations of Biological Change*

Prof. Anne Neville (School of Mechanical Engineering, Leeds), *Biomimetics - applying some principles from tribology*

Dr. Steve Howdle (University of Nottingham), *Putting the Fizz into Polymers - Polymer Synthesis and Polymer Processing using supercritical CO_2*

Dr. Mark Searle (University of Nottingham), *Insights into weak interactions in molecular recognition and self-assembly from peptide beta-sheets*

Dr. Benjamin Horrocks (University of Newcastle upon Tyne), *Self-assembled monolayers on hydrogen-terminated silicon surfaces*

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