

ORGANIC ELECTRONICS: INTERFACES, HETEROJUNCTIONS AND SEMICONDUCTOR DEVICE ENGINEERING

Richard Friend

Cavendish Laboratory
J. J. Thomson Avenue, University of Cambridge
Cambridge CB2 0HE, UK

Email: rhf10@cam.ac.uk

FETs, LEDs and photovoltaic diodes are routinely fabricated with molecular semiconductors and polymers, and are now developed as viable technologies for large-area flexible electronics. However, they also allow the study of the basic electronic excitations of this broad class of materials. I will illustrate the control of electronic structure that can be obtained at interfaces, including excitons confined to semiconductor heterojunctions for LED and photovoltaic operation, and electrons and holes confined to semiconductor-dielectric interfaces in FETs.

NANOMATERIALS BASED NANOTECHNOLOGY TO MEET THE 21st CENTURY TECHNICAL CHALLENGES

Paras N. Prasad

Institute for Lasers, Photonics and Biophotonics
Departments of Chemistry, Physics, Electrical Engineering and Medicine
State University of New York at Buffalo, Buffalo New York 14260

Email: pnprasad@acsu.buffalo.edu

Nanotechnology offers tremendous potential to meet 21st Century technical challenges in many areas of global priorities. These areas span from alternate energy, to healthcare, to environmental monitoring, to world security. Nanomaterials designed to contain multiple functionalities will play a vital role to meet the needs of this widely diverse range of applications. The coordinated manipulation of electronic, photonic, magnetic, thermal and structural properties in nanostructure and nanocomposite formulations can provide limitless applications for these materials. This talk will provide illustrations of multifunctionalities achieved in nanomaterials and their impact on the fields of world energy, health care and security.

The world faces a major challenge in meeting future energy needs; nanotechnology will provide new approaches for solar energy conversion, more efficient usages of oil and gas, as well as for energy storage. In areas of solar energy conversion, we are developing new nanomaterials based approach for efficient harvesting of solar photons over the entire solar spectrum and their efficient conversion to electrical energy. (e.g. direct or electrochemical conversion). The main objective is to enhance u.v. photon utilization by carrier multiplication derived from multiexciton generation as well as harvesting IR photons efficiently by nanocrystals, quantum dots, rods and multipods of a narrow band-gap semiconductor. Other areas of energy conversion and storage benefiting from multifunctional nanostructures includes CO₂ removal from natural gas for their more efficient utilization; nanocatalysts, nanoscale membranes in fuel cells; and nanostructured electrodes in solid-state batteries.

In the area of healthcare, we are developing multifunctional nanoparticles containing multiple imaging and sensing probes for in-vitro rapid detection of diseases and infections (such as bird flu, HIV, HPV, etc), together with a nanoplatform for multimodal-targeted therapy. These efforts will provide novel biotechnologies for health care, particularly in the new field of nanomedicine^{1,2}. The overall goal is to develop new nanomaterials platforms with the capability to detect diseases, deliver therapy and determine their effectiveness. We are using a nanoclinic platform for early detection of cancer which combines multimodal in-vivo imaging and targeted treatment using photodynamic, chemo, magnetic, radiation, thermal and gene therapies. Since this platform only targets cancer cells, collateral tissue damage is minimized. We are also applying nanoparticle based, non-viral gene/Si-RNA delivery to other major health care issues such as aging, genetic disorder, addiction and obesity.

In the area of world security, nanotechnology provides major advances in information technology, surveillance, security encoding, and chem/bio detection. For information technology, our program focuses on efficient high bandwidth and high density integration of optical communication using photonic crystal circuitry, and high capacity data storage using two-photon 3-D writing. A novel class of future nanomaterials for information technology and surveillance is metamaterials. For chem/bio detection, new nanoprobe, nanoplasmonic hierarchical structures, and periodic nanostructures are being developed and applied in a high throughput system for rapid detection.

This talk will conclude with a discussion of new opportunities for nanomaterials and nanoengineering in these fields.

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THE SYNTHESIS AND CHARACTERIZATION OF A SINGLE COMPONENT THERMALLY REMENDABLE POLYMER SYSTEM

Fred Wudl

Department of Chemistry and Biochemistry
Center for Polymer and Organic Solids and Materials Research Laboratory
University of California, Santa Barbara, CA 93106-5090, USA

Email: wudl@chem.ucsb.edu

In the field of structural materials, highly cross-linked polymeric solids are desirable due to their superior mechanical strength, durability and solvent resistance. In addition to these attributes, however, there also exist drawbacks: these materials experience a loss of re-cyclability and are usually brittle and rigid. Upon exposure to constant external stress, these systems experience thermal and mechanical fatigue that result in the formation of microcracks. When left untreated, these cracks propagate and enlarge through the sample, resulting in catastrophic failure.

A strong desire, therefore, exists to address the problem of microcrack formation and propagation before total failure of the system occurs. This has led to the recent development of re-mendable and self-healing polymer systems.¹⁻³ To allow for repeat mending cycles, it is advantageous to employ materials that incorporate the reformation of chemical bonds, such as the reversible Diels-Alder (r-DA) reaction. The energy required to break the DA adducts is much lower than the energy required to break the remaining covalent bonds in the molecule. This allows for rebonding of the intermonomer linkages after crack formation.³ In this work, we present a novel single component system that utilizes the r-DA reaction to achieve multiple cycles of mending. These materials are hard, colorless, and transparent at room temperatures, and can be custom-tailored to fit a range of desired working temperatures.⁴

Polymer specimens have been fabricated from the crystalline monomers, allowing for testing of mechanical properties both before and after fracture and healing cycles. In addition to possessing mechanical properties similar to many commonly used structural organic materials, these polymers also possess unique and interesting optical properties that are currently being investigated. While these materials are colorless and transparent after fabrication, they have been shown to fluoresce strongly in the presence of UV light. Additionally, these materials have shown birefringence when viewed between cross polarizers while under stress. The different colors observed are directly correlated to the amount of stress in the material, and the color pattern seen represents the distribution of stress throughout the sample. This unique feature of these polymer systems allows for the quantification of stress at specific locations in the sample before, during, and after fracture and healing events. While a specimen may appear to be completely healed due to the disappearance of a crack in the material, the birefringence would allow for any residual stress near the damage site to be observed. This would allow for a greater

understanding of the relative stress in the sample during a fracture event and throughout the healing process.

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THE EXCITEMENT OF CARBON NANOTUBES AND OTHER CARBON NANOSTRUCTURES

Mildred Dresselhaus

Department of Electrical Engineering and Computer Science
and Department of Physics
Massachusetts Institute of Technology
Cambridge, Massachusetts 02139, USA

Email: millie@mgm.mit.edu

There is much current excitement about the interesting advances in science and the unusual physical properties of carbon nanostructures, particularly carbon nanotubes and graphene, which are both of great interest at the present time. A brief review will be given of the physical underpinnings of carbon nanostructures that were developed over the past 60 years, starting with the electronic structure and physical properties of graphene and graphite, and then moving to graphite intercalation compounds which contained the first carbon nanostructures to be studied experimentally. Liquid carbon studies were precursors to the fullerene family of nanostructures and vapor grown carbon fibers were precursors to carbon nanotubes. Particular emphasis is given to the recent developments in our understanding of the photophysics of carbon nanotubes and graphene, with perspectives on future research directions for these fields and applications that are emerging.

LET THERE BE LIGHT ON PLASTIC SOLAR CELLS

K. S. Narayan

Jawaharlal Nehru Centre for Advance Scientific Research
Jakkur, Bangalore 560064, India

Email: narayan@jncasr.ac.in

Low cost clean-alternative energy source has become a necessity for sustaining the growth and quality of living in our planet today. The idea of photovoltaic PV cells based on carriers originating from thin polymer films, manufactured by printing and coating techniques from reel to reel, and packaged by lamination techniques is not only a novelty, but an attractive feature from commercial-environmental-design aspects. Recent efforts at our laboratory have addressed important issues in this growing field. The Donor-Acceptor system can be tailored to have a graded donor system where efficient energy transfer takes place within the donor system prior to the charge transfer processes with the acceptor system.¹ Realistic deposition conditions of the cathode lead to a variety of interfacial features, of which some are current limiting and detrimental. We realized the additional factor which can contribute to this low fill factors also can arise from the charge accumulation at the cathode-semiconductor interface.² We recently addressed issues related to the scaling trend of the efficiency as a function of electrode area and incident beam size.³ Our results also suggest routes to design higher performance large area solar grid structures taking these effects into account.³

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METALLIC GOLD IS MORE PRECIOUS ON THE NANOMETER SIZE SCALE; SOME PROPERTIES & APPLICATIONS OF GOLD NANOPARTICLES OF DIFFERENT SHAPES IN NANOPHOTONICS, NANOMOTORS, NANOMEDICINE AND NANOBIOLOGY

Mostafa A. El-Sayed

Laser Dynamics Laboratory, Georgia Institute of Technology
Atlanta, Georgia 30332-0400, USA

Email: mostafa.el-sayed@chemistry.gatech.edu

New fields such as optoelectronics, sensors, nanocatalysis, nanomotors and nanomedicine use the new exciting properties of gold and silver nanoparticles.¹ They possess the coherent localized surface plasmon oscillation when resonant Radiation interacts with their free electrons in the conduction band. This results in strong electro-dynamic surface fields that extends beyond the surface and enhance their absorption and scattering Radiative properties as well as of any system that falls within this field. We found that the interaction between the strong Plasmonic fields of two nanoparticles shifts their absorption wavelength according to a Universal Scaling law that can be used in determining the distance between sites in Biological systems (a new biological ruler).⁴ These surface fields are shown to affect the rates of physical and chemical processes like the relaxation of hot electrons in semiconductors⁵ and the retinal photo-isomerization⁴ primary step in Bacterio-Rhodopsin photosynthesis.

The strong scattering properties of gold nano-particles can be used in imaging and sensitive detection of cancer cells⁷. The strongly absorbed photon energy is rapidly converted into heat. This localized heating of the gold nanoparticles can lead to: their melting, the coherent oscillation of their lattice that can be used in Rapid light modulation; the rapid sublimation of their atoms leading to their propulsion and flying⁸ away with jet velocities or they can heat and melts attached cancer (or sick) cells leading to their destruction and thus used in in-vivo cancer therapy⁹.

These properties and examples of their applications will be presented and discussed.

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TAILORING NANOPARTICLES TO STUDY INTERACTIONS IN BIO-SYSTEMS AND DIAGNOSTICS USING RAMAN SPECTROSCOPY

Chandrabhas Narayana

Chemistry and Physics of Materials Unit, Jawaharlal Nehru Centre for Advanced Scientific Research, Jakkur, Bangalore 560064, India

Email: cbhas@jncasr.ac.in

Raman spectroscopy is a powerful technique in the hands of physicists and chemists since it provides vibrational fingerprints for chemically and biologically important materials. The Raman spectrum can be readily interpreted and used to identify specific chemical species in a mixture and to quantify their levels accurately. However, the Raman phenomenon is very weak and is only 1 Raman photon in 10^{6-8} incident photons. This has led to the restricted use of this potentially very powerful tool. The anomalous enhancement of Raman signals on a rough silver metal surface caused a great deal of excitement and subsequently similar discoveries were made with Ag and Au sols as well as thin films of these metals, which gave remarkable enhancements, which was later termed the surface enhanced Raman spectroscopy (SERS). Recent reports suggest an enhancement factor of 10^{14} due to surface enhanced resonant Raman scattering (SERRS), leading to the possibility of single molecular detection using SERRS similar to seen in fluorescence experiments. Rather than understanding fully this technique, chemists in diverse fields are continuing to study SERS and SERRS for its applications. It is therefore the application of these methods for chemical and bio-analytical applications that is catching the imagination of the scientists in all the fields.

Raman is a quantitative method and hence it is expected that SERS would also be used as a quantitative technique. Recent studies have shown that specific DNA sequencing can be done by SERRS. SERS as a detection method for bioanalytes, as a viable bioassay platform, the use of nanoparticle tags for in vivo imaging by SERS have all been demonstrated without any doubt. It has also been shown that SERS can be used for effective detection of a pathogens in extremely low counts. Based on the interfacial redox processes of proteins one could study the intracellular processes by SERS and hence could be used a potential single cell imaging tool. In doing all these as well as achieving the full potential of the SERS, there have been a lot of studies on the nanoparticles itself. It has been now becoming clear that there is a strong relationship between the SERS and the surface Plasmon resonance (SPR) of the nanoparticles and nanoparticle aggregates. Recent results indicate that if one tailors the nanoparticle aggregates to have SPR which is in resonance with the excitation wavelength as well as the absorption bands of the molecule being studied, one can achieve very strong SERS. It has also been shown that depending on the position of overlap of the SPR and the excitation wavelength and Raman bands, the intensities of the Raman bands vary in intensity. So one can tune the SPR of the nanoparticle aggregates to achieve optimum SERS enhancements.

To emphasize the effectiveness of SERS in biological systems, two examples have been chosen from our work, namely, study of drug protein interactions and viral load assay using SERS. We have effectively demonstrated on 300 kD full length protein like p300 the interactions of the protein with potential drugs and suggest the possible improvements in the drug to provide effective activation of the enzyme. Using the SERS, we have designed biomarkers to detect HIV viral RNA up to around 1000 counts using viral specific capture and detector oligo probes. In conclusion, SERS is turning out to be a probe which would develop both the methodology to develop newer SERS substrates and provide information to chemists and biologists which hitherto was inaccessible to them through other conventional probes like NMR, X-ray and CD spectroscopy.

ALTERNATIVE ROUTES TO MULTIFERROICS

C. N. R. Rao

Jawaharlal Nehru Centre for Advanced Scientific Research
Jakkur, Bangalore 560064, India

Email: cnrrao@jncasr.ac.in

Multiferroic are materials which possess both ferroelectric and ferromagnetic properties. Clearly, there is a contradiction here since ferromagnetism requires d-electrons while ferroelectricity generally occurs only in the absence of d-electrons. Several multiferroics demonstrating magnetoelectric coupling effects have, however, been discovered in the past few years, but they generally make use of alternative mechanisms in attaining these properties. Several new ideas and concepts have emerged in the past two years, typical of them being magnetic ferroelectricity induced by frustrated magnetism, lone pair effect, charge-ordering and local non-centrosymmetry. We shall examine multiferroic properties of BiMnO₃ in some detail. Charge-order driven magnetic ferroelectricity is interesting in that it would be expected to occur in a large number of rare earth manganites, Ln_{1-x}A_xMnO₃ (Ln = rare earth, A = alkaline earth), well known for colossal magnetoresistance, electronic phase separation and other properties. Magnetoferroelectricity has indeed been found in both bond- and site-charge-ordered manganates. In this presentation, we discuss novel routes to multiferroics, giving specific examples of materials along with their characteristics.

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NANOCATALYSIS ON NOVEL SUPPORTS: GRAPHENE SHEETS AND HIGHLY POROUS COORDINATION POLYMERS

M. Samy El-Shall

Department of Chemistry, Virginia Commonwealth University
Richmond, Virginia 23284-2006, USA

E-mail: melshal@vcu.edu

Nanocatalysis is a phenomenon of significant fundamental research and important practical applications in a variety of fields such as chemistry, physics, materials, environmental and atmospheric sciences in addition to its traditional significance in advancing the petroleum field. It encompasses supported or unsupported nm-scale metal catalytic structures (spherical nanoparticles, nanorods, nanoplates, nanocubes etc.) where the catalytic phenomena are specific to that length scale and, in general, are related to the high surface area and the density of the unsaturated surface coordination sites of the nanocatalysts.

In this talk, we present several examples of our work on nanocatalysis including vapor phase and microwave synthesis methods for supported nanocatalysts and the application of large surface area supports such as graphene and highly porous Metal-Organic Framework (MOF) polymers.

Graphene, a single hexagonally flat layer of graphite, has many unique properties including the highest intrinsic carrier mobility at room temperature of all known materials and very high mechanical strength and thermal stability. Graphene holds great promise for important potential applications in nanoelectronics, devices, development of new composite materials, and heterogeneous catalysis.

We will present a facile and scalable chemical reduction method assisted by microwave irradiation for the synthesis of chemically converted graphene sheets and metal nanoparticles dispersed on the graphene sheets. The method allows rapid chemical reduction of exfoliated graphite oxide (GO) using a variety of reducing agents in either aqueous or organic media. It also allows the simultaneous reduction of GO and a variety of metal salts thus resulting in the dispersion of metallic and bimetallic nanoparticles supported on the large surface area of the thermally stable 2D graphene sheets. We will present the catalytic activity of several metallic and bimetallic nanoparticle catalysts efficiently dispersed on the graphene sheets.

Metal-Organic Frameworks (MOFs) provide porous materials with a wide range of applications which includes storage, separation, sensing, and catalysis. We will present new results on the application of MOFs as efficient supports for a variety of metallic and bimetallic nanocatalysts. We will specifically focus on MIL-101, a chromium-based MOF that combines high surface area, mesoporous nature and stability in water in a unique way that makes this MOF a very attractive nanocatalyst support.

Finally, we will discuss the developments of new nanocatalysts supported on graphene and MOFs that combines high efficiency and selectivity for several important chemical reactions.

LITHIUM ION BATTERIES: MATERIALS ASPECTS AND PERSPECTIVES

B. V. R. Chowdari

Department of Physics
National University of Singapore
Singapore 117542

Email: phychowd@nus.wdu.sg

Rechargeable lithium ion batteries (LIBs) are one of the portable power sources that are extensively used in the mobile electronic devices like, cell-phones, notebook computers and digital camcorders. They employ lithium intercalation materials as the positive (e.g., LiCoO_2) and negative (e.g., graphite) electrodes and gel-polymer as electrolyte with Li ions shuttling between the electrodes during charge-discharge cycling. However, some of the materials that are being used in the present-day LIBs are toxic and expensive. Further, LIBs are relatively unsafe when used in large power-packs. Hence, extensive researches are being carried out to find new-novel materials with better performance and lower cost.

In recent years, nano-size particles and composites of electrode materials have been explored as viable alternatives to replace LiCoO_2 and graphite in LIBs. Specifically, anodes based on the tin (Sn) -oxides and composites, and formation-decomposition of lithium oxide (Li_2O) enabled by the nano-size metal (M) particles or a lithium-metal-oxygen matrix, 'Li-M-O' have been examined extensively for Li-cycling. Efforts are also being made to develop all-solid-state batteries with solid electrolytes.

After a brief overview of the current status of LIBs, results on selected systems of the recent work on the nanostructured-anodes from the Author's laboratory, viz., nano-size $(\text{V}_{1/2}\text{Sb}_{1/2}\text{Sn})\text{O}_4$, nano-size $(\text{Cd}_{1/3}\text{Co}_{1/3}\text{Zn}_{1/3})\text{CO}_3$, thin-film CoN, etc will be described and discussed to highlight that nano -science and -technology will greatly help in the development of future generation LIBs.

HETEROEPITAXIAL FORMATION OF SURFACE-PHASES AND SELF ASSEMBLED NANOSTRUCTURES

S. M. Shivaprasad

Jawaharlal Nehru Centre for Advanced Scientific Research
Jakkur, Bangalore- 560064, India

Email: smsprasad@jncasr.ac.in

The far-from-equilibrium process of epitaxial growth is strongly influenced by several kinetic factors that consequently provide a handle for the formation of novel superstructural phases. Among the several factors that influence heteroepitaxial growth aspects such as lattice mismatch, surface free energy difference and dangling bond density, play a crucial role in determining the initial stages of growth. I shall present some of my experimental experience in heteroepitaxial systems in which different kinetic factors play a dominant role, in the sub-monolayer regime.

The 7% lattice mismatched system of Ni on Ru(0001) surface shows pseudomorphic growth at lower coverages followed by the formation of misfit dislocations at higher coverages. The role of pre-adsorbed CO as surfactant in changing the Ni adsorption sites from the bulk stacking hcp to the weaker fcc sites is revealed by high resolution STM studies. The second system demonstrates the adsorbate induced reduction of surface free energy anisotropy of the atomically rough W(111) surface to the W(211) by forming pyramidal facets. Use of CO as a probe molecule in Thermal Desorption Studies of Pt on W(110) and W(111) manifest the surface morphological changes. Various systems are evaluated to identify the property that causes faceting. The dominant influence of dangling bonds on silicon surfaces is observed by the adsorption of non-reactive Ag, Sb and reactive Mn, Mg adatoms on planar Si(111), (100) and the faceted high index Si(5 5 12) surfaces. The ordered reconstructions of these clean silicon surfaces enable the formation of interesting and novel interfacial phases. On the Si(111) 7x7 surface the surface metallicity is shown to act as a barrier to Schottky barrier formation, while adatom nanowires and chains are formed on the dimer reconstructed Si(100) 2x1 and the trenched Si(5 5 12) surface, as observed by AES, LEED, XPS/XPD and EELS studies.

Overall, the presentation attempts to demonstrate the feasibility of the formation of self-assembled nanostructures with size and shape control, using the long range ordered misfit dislocations and surface reconstructions and dangling bond configurations, as templates for heteroepitaxial growth.

COMPLEX OXIDE THIN FILMS: FROM BASIC SCIENCE TO THERMOELECTRIC DEVICES

H.-U. Habermeier

Max-Planck-Institute for Solid State Research,
Heisenbergstr 1, D 70569 Stuttgart, Germany

Email: huh@fkf.mpg.de

Complex oxides with the perovskite structure can be found in almost every possible solid physical ground state with a variety of intriguing physical properties such as superconductivity at high temperatures, ferromagnetism, colossal magnetoresistivity, high thermopower and many more. Many of them are composed of transition metal oxides showing strong electron correlations. This can lead to a strong competition between lattice-, orbital-, charge- and spin ordering, all at similar energy scales. Developing a reliably technology to prepare single crystal-type thin films of these materials is seen as a cornerstone for future applications of complex oxides. In the talk a brief review of the related thin film technologies will be given with a focus on pulsed laser deposition, physics of thin film heterostructures and thermoelectricity in complex oxides thin films will be covered as case studies for fundamental research activities and application oriented work.

A first topic is to combine materials with different ground states (functionalities) such as superconductivity and ferromagnetism in the form of thin films and investigate their mutual interaction. At interfaces (substrate/film and filmA/filmB) the growth properties of complex oxides are governed by the constraint of preserving charge neutrality and stoichiometry imposed by the ionic character of the constituents. In this context the self-doping of interfaces - resulting from the modified charge transfer - could turn the interface between two insulators into a metal. Changes in the bonding characteristics at the interface may affect the spin properties because of the strong interaction between orbital and spin degrees of freedom. Furthermore, electronic reconstruction at the interface and broken lattice symmetry modifies orbital physics at the interface. Consequently the physical properties of an interface dominated sample will be different from those of its constituents. This concept opens a possibility for interface engineering and unexpected phenomena, which cannot be understood in terms of conventional band pictures, may thus appear. The combination of a ferromagnet and a superconductor is regarded as a prototype for this concept since these two ordering principles are antagonistic by nature and can not coexist in a homogeneous system. In this contribution the field will briefly be reviewed and recent results for charge transfer, orbital reconstruction and the different length scales for the interaction for YBCO/LCMO heterostructures will be given [1-3].

Second, complex oxides represent a new class of thermoelectric material with high thermopower and high thermal stability even at temperatures up to 1000⁰C. They are characterized by anisotropic Seebeck tensors and can be deposited onto substrates with a

vicinal cut in order to achieve atomic layer thermopiles (ALT). Early studies revealed that in $\text{YBa}_2\text{Cu}_3\text{O}_7$ thin films there appears a voltage when shining light pulses onto the surface of films which is of thermoelectric origin. Originally, only layered high T_c superconductor oxides have been regarded as suitable ALT materials; however, a similar effect was discovered in quasicubic LaCaMnO_3 thin films thus opening a new avenue for material systems other than high T_c superconductors for such experiments. Recently, research revealed that there are quite a number of complex transition metal oxides which demonstrate ALT properties, such as manganites, cobaltates and nickelates. In this contribution we explore the application potential of the concept of ALT for thermoelectric as well as photon sensing devices and pay special attention to designing novel materials with enhanced thermoelectric figures of merit. Furthermore concepts based on ALT materials are developed guiding to thin film thermoelectric power generation devices [4].

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FOLLOWING LOCAL STRUCTURAL CHANGES BY *IN-* AND *EX-SITU* NMR AND DIFFRACTION METHODS: APPLICATIONS TO BATTERY AND FUEL CELL MATERIALS

Baris Key, Rangeet Bhattacharyya, Hailong Chen, Frederic Blanc, Lucienne Buannic, Lesley Holmes and **Clare P. Grey**

Chemistry Department, Stony Brook University, NY 11794-3400, USA

Email: cgrey@notes.cc.sunysb.edu

The application of new NMR approaches to correlate local structure with function in materials used in batteries and in fuel cells will be described. For the batteries, we demonstrate that in-situ approaches allow processes to be captured, that are very difficult to detect directly by ex-situ methods. For example, we can detect side reactions involving the electrolyte and the electrode materials, and processes that occur during extremely fast charging and discharging. The approach will be demonstrated for the anode material silicon. Lithium-ion batteries (LIBs) containing silicon have been the subject of much recent investigation, because of the extremely large gravimetric and volumetric capacity of this anode material. This material undergoes a crystalline-to-amorphous phase transition on electrochemical Li insertion into crystalline Si, during the first discharge, hindering attempts to link structure in these systems with electrochemical performance. We apply a combination of static, *in-situ* and magic angle sample spinning, *ex-situ* ^7Li and ^{29}Si nuclear magnetic resonance studies to investigate the changes in local structure that occur in the actual working LIB. The first discharge occurs via the formation of isolated Si ions and smaller Si-Si clusters embedded in a Li-ion matrix; the latter are broken apart at the end of the discharge forming isolated Si ions. A spontaneous reaction of the lithium silicide with the electrolyte is directly observed in the *in situ* NMR experiments; this mechanism results in self-discharge, and potentially capacity loss, if Si-based LIBs are discharged to low potentials.

In a second example, we illustrate the use of a variety of different nuclei to investigate the nature of the defects in materials that have been proposed for use as oxygen-ion or protonic conductors in the electrolytes of solid oxide fuel cells. For example, BaZrO_3 can be doped with Y^{3+} to create oxygen vacancies. These vacancies can be filled with H_2O , the water molecules dissociating to form OH^- groups and H^+ , the OH^- occupying a vacancy and the H^+ coordinating to another oxide ion in the lattice. Both protons are then mobile, contributing to long-range ionic transport in these systems. We use a combination of multinuclear, single and double resonance NMR experiments to examine the local structure, the locations of the vacancies and how this affects protonic/oxygen ion motion in these systems.

NANOMATERIALS IN HETEROGENEOUS CATALYSIS

Robert Schlogl

Fritz-Haber-Institut der Max-Planck
Gesellschaft, Faradayweg 4-6, 14195, Berlin, Germany

E-mail: acsek@fhi-berlin.mpg.de

Catalysis is one of the most traditional areas in science and technology where nanostructuring plays a strategic role. Initially the quest for achieving high surface areas of precious active components was the driving force for developing strategies and synthesis concepts for nanostructured materials. During the last 3 decades a large number of observations on so-called “size effects” highlighted the critical need for nanostructuring catalysts. It is not only desirable but even essential for catalysts that a careful optimization of their nanostructure is performed. The conventional paradigm of nanoscience that the function of a material is optimized if its size is about equal to the size of the molecular functional unit (an active site in catalysis) does not explain the many practical observations. Attempts to tailor or design active sites as nano-objects did also not produce the expected breakthroughs in catalytic performance.

We have learned over the last decade that catalysts are dynamical systems adapting their chemical and geometrical structure to the chemical potential of their environment. Observable phenomena in catalysis material science indicating this process are sintering, segregation, lattice oxygen mobility, soot deposition and phase cooperation. Active sites are thus not pre-formed during catalyst synthesis but develop in the process of initial reaction of the synthesized pre-catalyst with the reactants under operation conditions. Such transformations occur under relatively mild conditions and are thus purely kinetically controlled. Nanostructuring is the most important optimization parameter allowing adjusting the solid-state kinetics with its dynamics to the reaction kinetics of the catalytic process.

An alternative approach is designing materials that are catalytically productive without undergoing transformations in feed gas; the chemical dynamics of the material should be disabled. Nanostructured carbon and intermetallic compounds are two classes of catalytic materials holding substantial potential both for mechanistic studies and for practical applications. They operate without detectable structural transformations allowing design concepts based on structure-function relations to be applied.

COMPUTATIONAL METHODOLOGIES FOR PROBING THE SELF-ASSEMBLY OF NANO MATERIALS

Michael L. Klein

Department of Chemistry, University of Pennsylvania
Philadelphia, Pennsylvania 19104-6323, USA

Email: klein@lrsn.upenn.edu

The talk will outline some recent developments in deriving so-called coarse grain (CG) models, which are being used in computer simulation studies of soft materials. The power of the CG-models will be illustrated by examining how the final structures (morphology) derived from the self-assembly of di-block co-polymers in solution depends on the molecular architecture of the polymer. The role of polydispersity will be discussed along with self-assembly in the presence of a hydrophobic substrate. The CG models will also be used to explore self-assembly of nanotubes at a liquid-liquid interface.

SMART DRUG DELIVERY SYSTEMS USING MULTIFUNCTIONAL NANOPARTICLES

Mamoun Muhammed

Functional Materials, Division
Royal Institute of Technology (KTH), Stockholm, Sweden

E-mail: mamoun@kth.se

Recent advances in the fabrication of nanoparticles allow a great control and the creation of novel and complex properties. Nanoparticle systems can be constructed with a number of constituents to provide several properties for a wide range of applications. Smart nanoparticle systems can be assembled to be responsive to external stimuli. Such systems can be especially useful for medical applications where they can be preprogrammed to respond to changes in external environment.

Multifunctional nanoparticles may be constructed of biocompatible matrix which can vary in size from few tens to few hundreds of nanometers. Poly lactic acid isomers have been a popular selection. Several components can be incorporated into the nanoparticles to achieve specific functions; e. g., reporters or visualization agents (MRI contrast agents, quantum dots) and superparamagnetic nanoparticles which can be used for magnetic targeting, visualization, heat generation, or localization of the nanoparticles to deliver their payload (drugs, genes, DNA) to given organ or tissues. More complex systems may also include components sensitive to external environment; e.g. temperature, pH, magnetic field, etc. The surface outer layer of the nanoparticles is constructed to be a conjugation platform to which several other molecules can be attached; e.g. targeting peptides, fluorescence compounds, etc., whereas the residual surfaces should be blocked in order to avoid undesirable binding to other molecules in the biological systems.

In this talk, we shall present a short review of some our recent results on some smart drug delivery systems of multifunctional polymeric nanoparticles and hydrogels responsive to temperature and external magnetic fields.

Recent Developments in Hybrid Inorganic-Organic Framework Materials

Anthony K. Cheetham

Department of Materials Science and Metallurgy
University of Cambridge, Cambridge CB2 3QZ, UK

E-mail: akc30@cam.ac.uk

The study of hybrid inorganic-organic frameworks is one of the most fashionable areas of materials science. The presentation will focus on some aspects of our recent work on hybrid framework, which may be nanoporous or dense. The synthesis of carboxylates and imidozalates will be described, and we shall examine the energetic and other factors that control structural trends in such materials [1-2]. We shall also examine some of the potential applications of hybrid materials in areas such as enantiomerically-selective catalysis, hydrogen storage, magnetism, photoluminescence, and multiferroics [3-6].

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