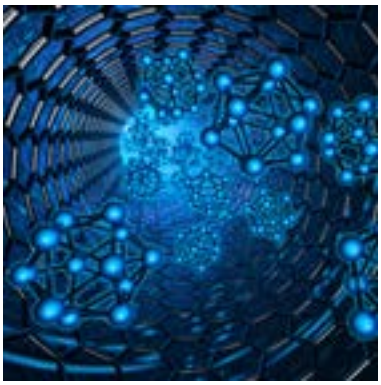
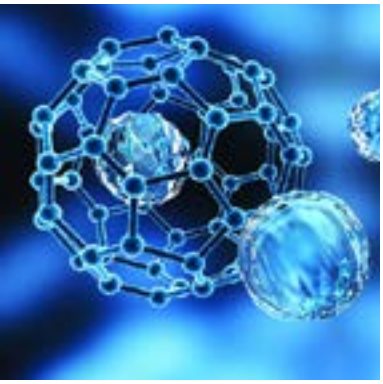
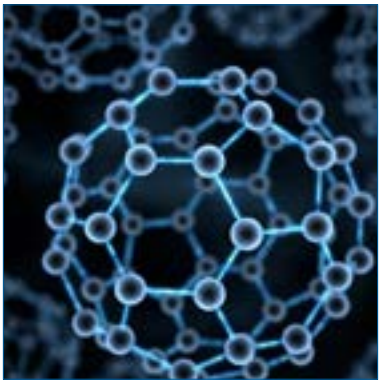
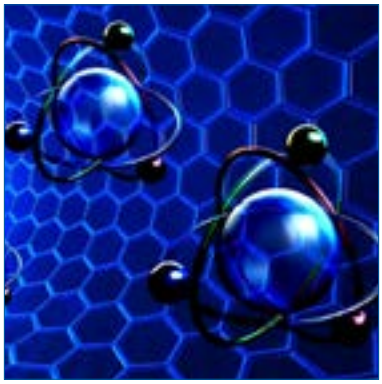
Poster Presentations

Nanochemistry 2017



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Conductive Ppy-DS/Fe-MMT layered nanocomposites

H Enomoto
Osaka Electro-Communication University, Japan

Conductive polypyrrole/montmorillonite (Ppy/MMT) nanocomposites were synthesized by the *in-situ* polymerization of Ppy in the gallery of MMT layers. The constrained environment of the interlayer gallery of clay host is expected to serve as a template within which a guest molecule is assembled, and to realize a high degree of polymer ordering. Fe^{3+} ions were intercalated into MMT gallery prior to the *in-situ* polymerization of Ppy. Sodium dodecyl sulfate (DS:Na) was adopted as a dopant of the conductive Ppy polymer. XRD patterns showed that all samples contain an organic polymer between all individual MMT sheets. Electrical conductivities are increasing with an increase of the basal-plane distance of nanocomposites, which indicates that the arrangement of Ppy polymer changes in the MMT gallery. The dc resistivity of Ppy-DS/Fe-MMT nanocomposites showed semiconductor-like temperature dependence. Through the variable range hopping (VRH) analysis, two-dimensional conduction is found to occur in Ppy-DS/Fe-MMT layered nanocomposites at lower temperature, although the pristine Ppy-DS polymer shows three-dimensional conduction. This is caused by two dimensional alignment of Ppy in MMT sheets, which suggests that the interlayer gallery of MMT serves as a template of Ppy arrangement.

Speaker Biography

H Enomoto has completed his Ph.D from Waseda University, Japan and Professor of Osaka Electro-Communication University (OECU), Japan. He was a Visiting Scientist of Oregon State University from 2000 to 2001. He has published more than 50 papers. He is a project leader of the Fundamental Electronics Research Institute of OECU.

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Fabrication and characterization of PEI/TaS2 LbL multilayer films

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PEI/TaS_2 LbL multilayer films were assembled by the layer-by-layer (LbL) technique from TaS_2 nanosheet colloids. The LbL technique is applicable to a wide variety of materials with charges, and is fabricated without special instruments. TaS_2 has a layered structure with negative layer charges. Li was intercalated into TaS_2 to prepare Li_xTaS_2. Exfoliation of TaS_2 was carried out by sonicating Li_xTaS_2 in water. Polyethyleneimine (PEI, MW=75000, 50 wt.% solutions in water) was adopted as cationic polyelectrolyte to assemble LbL multilayer films. The X-ray diffraction patterns shows that the (001) diffraction peak was observed at 9.6° (d=0.92 nm), which means the interlayer of TaS_2 was spread by 0.32 nm. Observed Δc=0.32 nm is almost as same as PEI monolayer. The calculated crystallite size from (001) diffraction peak was 12.2 nm. Since the thickness of one layer of the PEI/TaS_2 LbL multilayer film is about 1 nm, 12 nm is just equal to the LbL repeated times. The electrical characterization of PEI/TaS_2 LbL multilayer film will be discussed in details. .

Speaker Biography

M Irie is graduated from Osaka Electro-Communication University in 2014. She is a graduate student of Osaka Electro-Communication University.

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Assessment of the production of hydroxyl radical using nano zero-valent iron embedded in a mesoporous silica matrix

Steven Huezo
Desert Research Institute, USA

Zero-Valent Iron (Fe0) has been shown to detoxify water by creating hydroxyl radicals through Fenton-like reactions combined with hydrogen peroxide (H_2O_2) to get rid of organic contaminants. Nano-sized zero-valent iron (n/ZVI) in combination with oxidants and UV radiation, has been reported can increase the Fenton reaction rate and make water detoxification more effective. In this work, the production of reactive oxygen species, particularly hydroxyl radicals, was assessed for the heterogeneous photo-assisted Fenton-like reaction using nZVI embedded in a mesoporous silica matrix, hydrogen peroxide, and UV-A radiation. The experiments consisted of preparing a 10 μM solution of N, N-dimethyl-p-nitroaniline (pNDA, used as HO• radical probe) in 100 mL of water and adding the silica-embedded nZVI at three different loads (please include loads of Zvi in the SBA-15) with or without H_2O_2, and/or UV-A radiation (λmax=365 nm). The absorbance of the pNDA was measured and compared to that of clear, deionized water. The trials consisted of using immobilized nZVI alone, immobilized nZVI/H_20_2, and immobilized nZVI/H_20_2/UV. From the experimental results, we have seen that the best conditions for hydroxyl radicals production measured as pNDA bleaching are by the combination of immobilized nZVI/H_2O_2/UV despite nZVI, UV-A radiation and hydrogen peroxide alone were capable of bleaching pNDA to a certain extent. The use of the H_2O_2/UV system reached a plateau in hydroxyl radical production after 20 min of reaction. Two kinetic models are proposed to fit experimental data for the different reaction conditions tested and the obtained results were capable of fitting experimental data fairly good meaning that the proposed reaction mechanisms may occur within the reaction mixture to some extent. This novel material found was with interesting capabilities to produce reactive oxygen species, particularly hydroxyl radicals, under photo assisted conditions and high potential for further photocatalytic applications in water treatment.

Speaker Biography

Steven Huezo Pineda is an assistant researcher working with Erick Bandala at Desert Research Institute in Las Vegas, Nevada. He is an undergrad majoring in Biochemistry at the University of Nevada, Las Vegas. He has been working at DRI (Desert Research Institute) since January, focusing on Zero-Valent Iron and using it to clean pollutants of water. Steven Huezo will plan to continue his work next year, working with the Department of Energy to clean chlorine from groundwater.

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Accepted Abstracts

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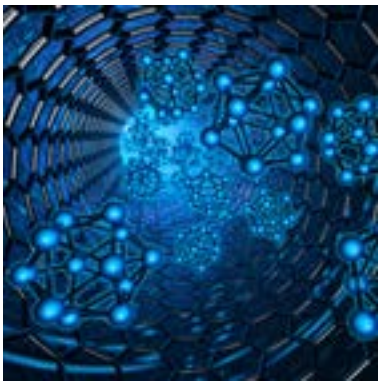

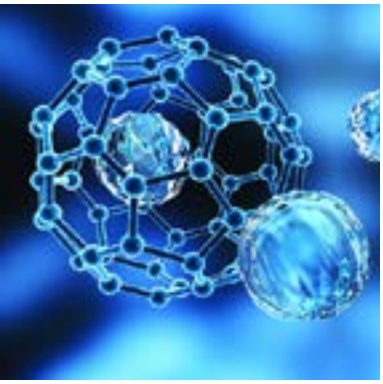
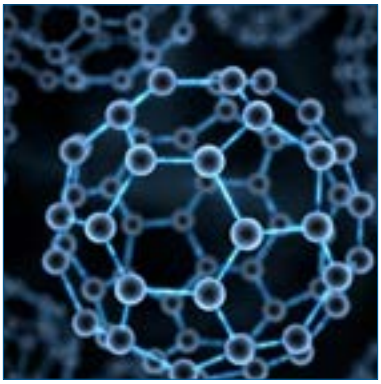
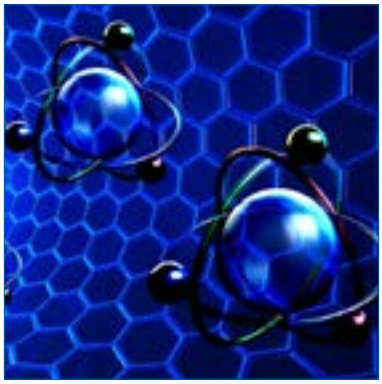

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Metal and metal oxide nano-particles on quasicrystalline surface: A notable catalytic application in green energy

T P Yadav
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Quasicrystals are complex in nature and it has been difficult to gain atomic scale understanding of catalytic activity of leached quasicrystals. Additionally, the underlying role of quasicrystals in the catalytic activity is yet to be understood. In order to achieve this information, we have attempted to create a simple model catalyst of nano particles on quasicrystalline surfaces by leaching well defined surfaces of single grain quasicrystals. As the first step of these studies, we present here the effect of leaching treatments on surface morphology and chemical composition of different Al-based quasicrystals studied by scanning electron microscopy (SEM), energy dispersive X-ray (EDX) analysis and X-ray photoelectron spectroscopy (XPS). The high symmetry surfaces of single grain icosahedral (i)-Al-Cu-Fe and decagonal (d-) Al-Ni-Co, (d)Al-Cu-Co quasicrystals and a polygrain (i)-Al-Pd-Re, (*i*)-Al-Cu-Fe, (*i*)-Al-Pd-Mn quasicrystal with random surface orientation were leached with NaOH solution at varying times and the resulting surfaces were characterized by scanning electron microscopy, energy dispersive X-ray analysis and X-ray photoelectron spectroscopy. The leaching treatments preferentially remove Al producing nano-particles of the transition metals and their oxides. The leached fivefold surface of i-Al-Cu-Fe exhibits micron sized dodecahedral cavities on which the nano-particles are precipitated. However, no specific microstructure has been observed on the tenfold surface of d-Al-Ni-Co and the polygrain i-Al-Pd-Re. Quasicrystalline surface can be regained after polishing the leached layer, indicating that leaching occurs only in a limited depth from the surface. The 2 hour leached as grown and mechanically activated Al-Cu-Fe alloys was subjected for catalyst application in hydrogen storage materials. The catalytic effect of leached alloy on the de/rehydrogenenation characteristics has been studied. The hydrogenation behavior including absorption kinetics will be discussed and presented in detail.

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Development of nanoparticles loaded transdermal patches of tenoxicam

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Tenoxicam (TX) is NSAID indicated to treat rheumatoid arthritis but possess poor solubility, GI irritation and first pass effect. Hence in the present work it was initially made as nanoparticles to facilitate absorption and at later stage nanoparticles loaded transdermal patches were developed using promising nanoparticles of tenoxicam. Nanoparticles were prepared with chitosan by ionic-gelation technique Trail formulations such as F1 to F5 were prepared by using 0.25% w/v sodium TPP and different concentrations of chitosan (0.5%,1%, 1.5%,2% and 2.5%,w/v). These formulations were evaluated for percent drug content, and % drug release and mean particle size by zeta sizer. They were evaluated by percentage drug content, in-vitro release, particle size, zeta potential, DSC and FTIR analysis. Percentage drug content values were in acceptable range of 99.1 -99.8%. All formulations were produced in nanosizes and the sizes are 101.10nm, 108.7nm, 178.30nm, 314.3nm, and 923.2nm for F1, to F5 in sequence. DSC and FTIR analysis indicated there is no interaction between the drug and polymers. Among them F4 having mean particle size 178.30nm and zeta potencial of 35.5 mV45 was considered as pomising formulation. Transdermal patches of TX were prepared by solvent casting method using different ratios of polymers HPMC, E.C, and PVP. Chloroform: methanol (1:1) was used as solvent. Dibutyl phthalate and propylene glycol were added as plasticizer and permeation enhancer respectively. Three formulations were obtained with optimum properties in terms of percentage drug content (98.56%-99.88%), thickness (1.7mm±0.03 to 1.3mm±0.021 surface pH (6.5 to 6.9), folding endurance (191 to 200). Ex- vivo permeation studies of a patch (TT6) containing HPMC K400M 880 mg EC, 270 mg and PVP 260 mg exhibited optimum drug release of 99.51% in 60 min.

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Heterogenous graphene supported cobalt metal catalyzed dehydrogenation of N-heterocyles

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The promoterless AD (acceptorless dehydrogenation) reaction with the release of H_2 provides promising synthetic routes for several organic transformation such as alcohol dehydrogenation to carbonyl compounds as aldehydes, ketones, esters, amides, amine to imine and N-heterocycles dehydrogenation which is synthetically very important. Dehydrogenation of N-heterocyles were mediated by cobalt heterogenous has been done at atmospheric condition with the liberation of hydrogen which is most atom efficient way to produce quinoline. Owing to the increasing demand for environmentally benign synthetic processes, promoterless AAD reactions are desirable. Conventionally, oxidative dehydrogenation reaction has been performed using stoichiometric or excess amounts of oxidants such as DDQ, peroxides, iodates, chromium(IV) reagents and metal oxides, that produce large excess of hazardous waste equivalent to the oxidants which is undesirable environmentally and economically. An alternative to these strong and toxic oxidants is to use pressurized oxygen air or oxygen which can cause explosion hazards. Removal of dihydrogen atoms from adjacent atomic centers of organic molecule is highly thermodynamically uphill process. Thus, it would be challenging to explore the catalytic performance of hetrogenous catalysts for the dehydrogenation of nitrogen heterocycles. Our interest is in the development of efficient heterogeneous catalyst containing sustainable transition metals, such cobalt for the dehydrogenation reaction. we have propse first cobalt based heterogenous catalytic system for challanging catalytic dehydrogenation reactions of nitrogen heterocycles. In this reaction only hydrogen is side product which is good in the context of 'hydrogen economy' and is an effective alternative to the classical oxidation reactions.

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Aminophenyl double-decker shaped silsesquioxanes: Physical, thermal characterization and applications

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A recently developed class of nano-structured, cage-like silsesquioxanes, formally known as double-decker shaped silsesquioxanes (DDSQ), offers the opportunity to form hybrid polymers with silsesquioxane cages as a part of the polymer backbone. Unlike functionalization of trisilanol silsesquioxanes, functionalized DDSQs generate *cis* and *trans* isomers with respect to the Si-O core. Therefore, it is logical to characterize physical and thermal properties of mixtures with different ratios of *cis* and *trans* isomers. Moreover, these characteristics are also relevant when reacting or incorporating these isomers, or mixtures thereof, with other molecules to form novel materials. In this study, three aminophenyl DDSQs were synthesized. More specifically, two meta-aminophenyl DDSQs, which were differentiated according to the moiety attached to the D-Si (methyl or cyclohexyl), and one para-aminophenyl DDSQ with a methyl moiety were used. Chemical, physical, and thermal characteristics were evaluated for individual isomers as well as binary mixtures of different *cis*/*trans* ratios. Phase diagrams representing solid-liquid melt equilibria of the binary *cis*/*trans* mixtures were developed. Single crystal X-ray diffraction data of isolated isomers helped to interpret the phase behavior. A specific application was chosen to demonstrate advantages of using these DDSQ in high performance thermosetting oligoimides over their organic counterparts. Specifically, they exhibited advantages in areas of liquid to solid *trans*ition and viscosity, which greatly expand the processing window. Additionally, they improve oxidative stability and reduce moisture uptake which provided a significant enhancement for service reliability.

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Filled and empty orbital interactions in a planar covalent organic framework on graphene

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The electronic characteristics of a planar covalent organic framework (COF) on graphene are investigated by means of dispersion-corrected density functional theory. The aromatic central molecule of the COF acts as an electron donor to graphene, while the linker of the COF acts as an electron acceptor. The concerted interaction between the filled orbitals of the central molecule and empty orbitals of the linker promotes the formation of planar COF networks on graphene. The calculation results are in very good agreement with experimental findings of an ordered hexagonal and square COF planar on graphene, which sheds light on the super molecular assembly mechanism.

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Regime of gene silencing: Efficient siRNA delivery into cancer cells using nanocapsules

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RNA interference and the therapeutic applications using small interfering RNA was discovered more than 10 years ago and currently is used in various applications including cancer theragnostic. However, the research in this field is still in its infancy. Many challenges like safe delivery of targeted siRNA to nucleus and cytosol of cancerous cells without compromising the activity of siRNA needs to be addressed. We have overcome this hurdle with the help of nanotechnology using PLGA hollow NPs (PLGAHNPs) and suppressing the oncogene of MYC transcription factors by using anti myc-siRNAs in human cancer cell lines. siRNA was encapsulated in PLGAHNPs. PLGAHNPs of size 70 nm had high efficiency of gene release at pH 4.2 under in vitro conditions. Cell penetrating peptide (CPP)- Tat peptide (TAT) and peptide nucleic acid nucleolus localizing signal (PNA-NLS) was used for siRNA delivery without interrupting the therapeutic activity of siRNA. Incubation of the siRNA encapsulated PLGAHNPs functionalized with TAT and PNA-NLS (TAT-siRNA-PNA-PLGAHNPs-siRNA) with cancer cells resulted in reduced cell proliferation. A downregulation of gene expression by 90% was observed even with low concentration of siRNA. We found complete arrest of cell division which was mediated by downregulation of MYC expression. Further we used the combination of gold nanoparticles with PNANLS and siRNA encapsulated in PLGAHNPs around the mean size diameter of 100nm. The encapsulation efficiency of siRNA with AuNPs is increased by 20% when compared to siRNA alone in PLGAHNPs. The gene expression of MYC in cancer cells was down regulated by 92%.

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Technology of nanofabrication of GaN-based substrates for surface enhanced Raman spectroscopy measurements: Chase for hot-spots

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It is commonly accepted that the presence of so-called hot-spots is necessary for obtaining high enhancement factor (EF) of Raman signal from individual molecules attached to the plasmonic metal particles. The hot-spots contribute most significantly to the overall SERS intensity. Two approaches are usually used in order to deliver SERS platforms, namely planar and nano-structured substrates, both with plasmonic metal particles on the top surface. The aim of this presentation is to review the new technology of nano-structuring of hetero-epitaxial GaN layers. The nano-structures are formed using galvanic, electroless and orthodox etching methods. The principles of etching methods, commonly used for revealing and analysis of crystallographic and electrically active defects, will be discussed. As a result of studying defects in hetero-epitaxial GaN, the nano-structured hetero-epitaxial GaN surfaces appeared to be suitable for SERS measurements. It will be shown that the dislocation-related nano-pillars and pits (formed during electroless and orthodox etching, respectively) are responsible for formation of hot-spots and the increased EF. Tailoring of plasmonic metal layers sputtered on etched GaN surfaces for increased SERS efficiency using dealloying and annealing will be also addressed. The novel SERS platforms based on etched GaN show very good mechanical and chemical stability and high EF up to 10^6 for the examined molecules of para-mercaptobenzoic acid (pMBA) and pyridine. This feature enables also time-lapse measurements of various biological systems such as Hepatitis B virus antigen and different bacteria (BC, BT, BS).

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Synthesis of carbon nano-spheres by thermal plasma treatment of polypropylene

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In the last century, nano-structured carbon materials have attracted considerable attentions due to their multiple beneficial applications. These carbon nano structures have been synthesized by different technologies including laser ablation, chemical vapor deposition (CVD), plasma enhanced chemical vapor deposition (PECVD), etc. Due to operation in atmospheric pressure and being used for conversion the abundant low value materials such as solid municipal wastes to very useful materials, thermal plasma is one of the most appropriate methods for carbon nano-structured synthesis. In this study, it has been experimentally demonstrated the feasibility of producing carbon nano-spheres (CNS) from common plastic waste material (polypropylene), using thermal plasma treatment. Samples were treated in a furnace fitted with a twin dc thermal plasma torch. The resultant solid products were analyzed to determine their composition and morphology by EDS and SEM analysis. The EDS pattern for the samples synthesized at 80 A illustrates that there are some kinds of impurities in solid products such as oxygen and aluminum which came from vaporization of torch's alumina ceramic nozzle. However, in the pattern obtained at 100 A, there was just one major carbon peak. The elevated temperature plasma jet at 100 A arc current can vaporize all the contamination from sample and processing region, and separate them from conclusive solid products. The SEM image for 100 A treatment reveals that the solid carbon particles are very fine carbon nano-spheres with about 50 nm diameter. This method for synthesis of carbon nano-spheres may find a way to be considered in industrial waste disposal installation, since these advanced products can be obtained from very non-useful and environmentally hazardous materials which may enhance the economic efficiency of plasma waste disposal industry, significantly.

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III-nitrides: A universal semiconductor for energy applications thermoelectric and solar cells

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The development of wide-band gap compound semiconductor materials and structures has been led by the III-nitrides and they are fueling a revolution in solid state lighting, solar cells, thermoelectric and other applications. The talk will review many of the contributions that the III-nitrides have made to date before focusing on the development of InGaN for high temperature thermoelectric materials and a new generation of high efficient solar cells. Specifically, we will talk the various approaches to increase thermoelectric efficiency of III-nitrides, including electron quantum confinement, and phonon scattering to increase the power factor and decrease the lattice thermal conductivity. Additionally, high density-of-states (DOS) by size reduction, resonant states by impurity doping, and multi-valley band structure by band degeneracy have been utilized to further enhance its figure of merit (ZT) value. The impact of doping, and crystallographic defects on electrical and thermal properties on the TE properties of nitride thin films grown by metal organic vapor deposition (MOCVD) will be systematically analyzed. Additionally, we will talk the III-nitrides for a new generation of highly efficient solar cells. For instance, InGaN with indium compositions up to 30% have been developed for photovoltaic applications by controlling defects and phase separation. InGaN solar cell design involving a 2.9 eV InGaN p-n junction sandwiched between p- and n-GaN layers yield internal quantum efficiencies as high as 50%; while devices utilizing a novel n-GaN strained window-layer enhanced the open circuit voltage. These results establish the potential of III-nitrides in ultra-high efficiency photovoltaics.

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Potential of strained SnO_2 as a photo-catalyst for water splitting process

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Photocatalytic water splitting technology has recently received extensive attention as a promising method to produce hydrogen, which has generated an urgent need to find alternative photocatalytic materials for such technique. In the present study, the electronic and photocatalytic properties of SnO_2 under uniaxial strain have been examined, based on density functional theory (DFT), showing that under tensile strain the band gap energy decreases, while an opposite behavior is demonstrated in the case of compression. Band edge alignments of unstrained SnO_2 shows that the VBM is more positive than the redox potential of O_2/H_2O (1.23V) while the CBM for pH = lies above the redox potential of $H+/H_2$ (0V), which mean that the pure SnO_2 cannot be used for hydrogen evolution reaction (HER). Applying compressive strain, the CBM edge position decreases gradually as the strain percent increases, in other hand under tensile strain the CBM edge position could be corrected for pH ≥ 10 which clearly reveals the ability of mechanical strain to modulate the band structure and the photocatalytic properties of SnO_2 in order to improve its suitability as a photo-catalyst for water splitting.

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Thermodynamic analysis of nano particle ceria-based oxides at elevated pressure for solar thermochemical redox cycles fuel production

Bahram Sadaftar
KTH Royal Institute of Technology, Sweden

The thermodynamics of nano-ceria-based metal oxides have been studied in the context of solar thermochemical redox cycles for splitting H_2O and CO_2 at elevated pressure. Because of the resistance to high temperature of nano-ceria-based metal oxides $MxCe1-xO_2$, such systems are suitable for resolving stability problems frequently encountered with high-temperature operations. Catalytic systems for CO_2/H_2O conversion, with Gd, Y, Sm, Ca, Sr, nano-particle ceria-based perovskite, were synthesized, and tested at close to industrial conditions at the Royal Institute of Technology in Stockholm. Oxygen nonstoichiometric was investigated at high temperatures, pressure for a redox system. Subsequently, relevant thermodynamic parameters were computed and equilibrium H_2 and CO concentrations determined as a function of reduction conditions (T, PO_2) and ensuing oxidation temperature. At 8 bar and above 1073 K, the degree of reduction is positive for pure nano-ceria particle. As a result, at a given reduction temperature and elevated pressure, more H_2 and CO is generated at equilibrium state.

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Pulsed submerged arc nanoparticle synthesis, disinfection and decontamination

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Generating a pulsed submerged arc (SA) within a liquid produces a plasma bubble comprised of ionized material evaporated from the electrodes and the liquid. This plasma bubble serves as a microplasma reactor in which radiation, active chemical species, and nano-particles are produced. The arc discharge may be initiated by high voltage breakdown, or by mechanically breaking contact between current carrying electrodes and drawing an arc; the initiation method influences the type of particles produced and the energy expended. Micro- and nano-particle production was studied using pulsed arcs submerged in ethanol and water. Drawn arc initiation tended to produce a larger proportion of micro-particles than with breakdown initiation. The micro-particles tended to be comprised mostly of the electrode material, while nano-particles tended more to incorporate material from both the electrodes and the liquid. Particularly interesting were: (a) Ni nano-particles produced with Ni electrodes in ethanol, in which the Ni was supersaturated with dissolved C, and enveloped with a protective C outer layer, and (b) pure C nano-particles produced with graphite electrodes in ethanol, including nano-onions and magnetic C nano-particles. UV radiation and OH radicals produced by the SA disinfected water was inoculated with E. coli bacteria. Treatment of 50 ml of water containing 2×104 c.f.u./ml of bacteria for 5s with 48 mJ pulses applied at a 100 Hz repetition rate produced a survival rate of <5×10-4 with an energy expenditure of 0.14 kW-hr/m^3. Water contaminated with various organics, including Methylene Blue (MB), Sulfadimathoxine (SDM) antibiotic, phenol, and effluents from various industrial plants, was treated with a drawn arc initiated SA using C, Fe, Ti, and Cu electrodes, and their combinations, both without and with the addition of (0.01-0.5%) H_2O_2. The treated solutions were examined by Raman and absorption spectroscopy. Particles produced during the arc treatment were studied by SEM, XPS and XRD. It was found that MB was decomposed both during and after arc treatment. The produced nano-particles defined the character of the pollutant removal and the level of the removal ratio after SA treatment. With C electrodes, the MB concentration exponentially decreased for the duration of the treatment, while with the other electrodes the MB concentration saturated. The saturation is explained by a decrease of the oxidative species concentration with SA treatment time for these electrodes. Aging of the solutions after the SA treatment with all combinations of electrodes in the presence of H_2O_2 removed ~99% of the MB contaminant. The decomposition during aging may be associated with the accumulation of oxidative species, particularly peroxides, on the surface of eroded particles that gradually oxidized the MB. The association of particles with the decomposition of impurities is supported by faster decomposition in cases where the particle diameters were smaller. An MB decomposition yield of G99.6=90 g/kWhr was obtained using SA with Ti and Fe electrodes and 0.5% H_2O_2 addition. SA was successfully applied to treating industrial waste water from a pharmaceutical plant and decomposing phenol dissolved in water.

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Identifying noble factors and their functions in DNA damage response pathway

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To prevent genomic instability disorders, cells have developed a DNA damage response. The response involves various proteins that sense damaged DNA, transduce damage signals, and effect DNA repair. Among various types of DNA damage, double-stranded breaks are highly toxic to genomic integrity. Homologous recombination (HR) repair is an essential mechanism that fixes DNA damage because of its high level of accuracy. Although factors in the repair pathway are well established, pinpointing the exact mechanisms of repair and devising therapeutic applications requires more studies. RAP80 is one of key molecules in DNA damage response pathway. This protein localizes to sites of DNA insults to enhance the DNA-damage responses. I identified TRAIP/RNF206 as a novel RAP80-interacting protein and found that TRAIP is necessary for translocation of RAP80 to DNA lesions. Biochemical analysis revealed that the N terminus of TRAIP is crucial for RAP80 interaction, while the C terminus of TRAIP is required for TRAIP localization to sites of DNA damage through a direct interaction with RNF20-RNF40. My research demonstrated that the novel RAP80-binding partner TRAIP regulates recruitment of the damage signaling machinery and promotes homologous recombination.

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Fabrication of CVD graphene-based kelvin sensor for online scale monitoring system

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CVD graphene is an ideal candidate for a new class of sensor systems, which were not possible before. This is due to its 2-d nature (inert, conductive where the conductivity can be modulated when exposed to various ions, molecules, and gases). Also, Graphene is mechanically very strong yet flexible so that it can be applied on various shapes and forms; in addition to its tolerance to high temperatures (stable till 700 °C). Furthermore, the electrical characteristics of the graphene changes when chemical molecules in the surrounding covalently or non-covalently interact with the graphene. These molecules act as dopants that shift the fermi energy of the graphene. The goal of this work is to fabricate a kelvins structure like sensor with a graphene mat as an active material between four metal pads made of Aluminum over titanium. In this study graphene sensor device based on kelvin structure is fabricated to detect NaCl salt in water solution. The successful operation of such a sensor opens a path to utilizing graphene-based devices for monitoring other scales, including $CaCO_3$ and $BaSO_4$ which are common for scale precipitation in the oil industry. The used graphene is grown in our lab on a copper foil, transferred to sensor structure and used as a sensing material. The electrical response of the fabricated sensor is studied by means of measuring changes in the electrical resistance before and after using the NaCl salt solution.

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Comparative study on patterns of rounded concave and convex objects achievable via integrated lithography realized by circularly polarized light

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Comparative study has been performed on the spectral and near-field properties of concave and convex nano-object-patterns that can be fabricated via colloid-sphere lithography (CSL) and via interferometric illumination of colloid sphere monolayers (IICSM) by applying circularly polarized light. Previous studies on hole- and disk-arrays in the literature have shown that the s/p-polarized transmittance on the former corresponds to the p/s-polarized reflectance on the latter type of patterns, according to the Babinet principle. In CSL hexagonal pattern of nano-ring and nano-crescent shaped holes can be prepared via illuminating a hexagonal monolayer of Au colloid spheres by perpendicularly and obliquely incident circularly polarized beams, as a result two and four geometrical parameters can be tuned independently. In IICSM mini-arrays composed of a central ring and satellite nano-crescents can be fabricated via illuminating a hexagonal monolayer of Au colloid spheres by two interfering circularly polarized beams, and six geometrical parameters (p pattern period, t nano-object distance, d nano-ring and nano-crescent diameter, ε nano-crescent opening angle and ω orientation) can be tuned independently (Fig. 1a, b). When the Au colloid sphere monolayers are aligned on thin Au films, nanoholes of various shape can be directly fabricated, while a lift-off procedure makes it possible to transfer the pattern into analogous convex nano-objects. Both of the concave and convex hexagonal patterns of nano-rings and nano-crescents, as well as of the two different (p=300 nm and p'=600 nm) rectangular patterns of mini-arrays were re-illuminated by p-polarized light in different azimuthal orientations to demonstrate their spectral engineering capabilities. Our results have shown that in complementary complex patterns illuminated by complementary beams the reflectance and transmittance are interchanged. The convex patterns indicate the cavity resonances of individual nano-objects and the lattice resonances on their array, while the optical response of the concave patterns is more structured due to the Fano modulations originating from coupled localized and propagating modes. The spectra on the hexagonal pattern of nanorings did not show azimuthal orientation dependence, while the spectra on the hexagonal pattern of nano-crescents and on both rectangular patterns composed of analogous miniarrays strongly depend on the azimuthal orientation. The hexagonal pattern of nano-rings indicates the "U-resonance" of crescent-shaped objects, which is independent of the E-field oscillation direction due to their symmetry properties. In contrast, on the hexagonal pattern of nano-crescents the convex reflectance in γ=0°/90° corresponds to the concave transmittance in γ=90°/0° azimuthal orientation (Fig. 1c). Similarly, on the rectangular pattern of mini-arrays the convex reflectance in 30°/120° azimuthal orientation corresponds to the concave transmittance in γ=120°/30° (Fig. 1e). On both rectangular patterns of miniarrays at small wavelength analogous extrema are observable, while the larger periodic rectangular pattern exhibits additional extrema at larger wavelengths. The charge distribution and corresponding near-field indicates U / C1 and C2 resonance on the convex hexagonal array of nano-crescents in γ=90°/0° azimuthal orientation, while on the convex rectangular pattern analogous resonances appear in γ=30°/120° (Fig. 1d, f). However, the charge and near-field distribution on the complementary concave pattern is perturbed by coupled localized and propagating modes.

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Plasmonic properties of Al nano-concave arrays

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Surface plasmons (SPs), excited by the interaction between light and metal surfaces have attracted great scientific interest due to their ability to enhance light emission from solid-state materials. Among metals used in surface plasmon coupled luminescence, Al gains increasing attention owing to its advantageous plasmonic properties in the UV region related to a small imaginary part of its relative permittivity at the UV wavelength range, low cost and abundance. In this talk, plasmonic properties of regular arrays of Al nano-concaves with various pitch size prepared by anodization of Al, will be presented. As a proof of concept, the enhancement of UV emission from ZnO thin films deposited on the Al nano-concave arrays and the modulation of the enhancement factor by the distance between the Al nano-concave centers will be shown. Zinc oxide (ZnO), with a wide direct band gap (3.37 eV) and a large exciton binding energy (60 meV), has been considered as a promising candidate for efficient ultraviolet (UV) light-emitting devices (LEDs) and low threshold UV lasers. For photonic applications of ZnO it is of outmost importance to obtain highly efficient UV emission from the near band edge (NBE). Plasmonic enhancement of the UV emission by Al nanostructures is a promising way to achieve this goal.

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The progress of nano metallic drug conjugate in cancer chemotherapy

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Metallic drug nano conjugate chemistry is an interdisciplinary thrust area of cancer biology research; is currently much more known for its many applications in drug delivery and also has enormous potential to act as diagnostic agent. Development of new drug design and therapeutic strategies that could target cancer cells leaving normal cells unaffected still continues to be a challenge. Series of new metallic drug nano conjugate were designed, synthesized and characterized by, TEM, SEM and various spectroscopic methods. *In vitro* DNA binding studies of the compounds investigated by absorption and emission titration methods which revealed that compounds recognizes the minor groove of DNA in accordance with molecular docking studies with the DNA. Gel electrophoretic assay demonstrates the ability of compounds to cleave pBR322 DNA through hydrolytic/oxidative process which was further validated by T4 religation assay. To understand the metallic nano drug–protein interaction of which ultimate molecular target was DNA, the affinity of compounds towards HSA was also investigated by the spectroscopic and molecular modeling techniques which showed hydrophobic interaction in the subdomain IIA of HSA. Furthermore, nano conjugate showed high inhibitory activity against Topo-Iα suggesting that new nano conjugate is an efficient DNA cleaving agent. *In vitro* studies on the anticancer activity against the cancer cell lines revealed that nano conjugates have the capability to kill the cancer cell. The efficiency of new nano conjugates is higher than the earlier reported.

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Smart targeted erlotinib-SPION nanoparticles for MRI applications

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Despite the success erlotinib achieved in fighting lung cancers, the problems of grading and monitoring the tumor as well as predicting the treatment response may result in failure of the therapy and resistance of the tumor, which requires the use of a suitable diagnostic tool that can monitor the treatment and predicting the treatment response. As an attempt to address such problems, we designed a novel theranostic nanoparticle formulation (NPs) of superparamagnetic iron oxide core, coated with a thin dextran layer (as determined by transmission electron microscope (TEM) imaging and dynamic light scattering) and linked to erlotinib. Such NPs are smart, targeting cancer cells that overexpress the EGFR, releasing the active drug intracellularly rather than in the blood stream, accumulating inside the cancer cells producing high contrast in the magnetic resonance imaging (MRI) and being non-toxic to the EGFR-negative cells. Cellular uptake of the NPs was higher than the product used commonly in clinical practice as MRI contrast agent, this was evident from the MRI, TEM and Prussian blue imaging results. Furthermore, we tested the molecular mechanisms that may account for the potent activity of our NPs and found that the NPs inhibited the phosphorylation of the overexpressed EGFR as well as the oncogenic signaling pathways downstream of the EGFR such as the ERK and NF-κB pathways which was confirmed by Western blotting and confocal immunocytochemical imaging. Moreover, the T2-weighted MRI images of the BALB/c nude mice showed significant decrease in the normalized signal within the tumor post-treatment with the NPs compared to the non-targeted control iron oxide nanoparticles.

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Studies on different SnO_2 nanostructures for VOC gas sensing

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Semiconductor oxides are a very important class of materials because they possess excellent properties and have seen wide application in various areas of science and technology like solar energy conversion, photo catalysis, gas sensors, and optoelectronics. They have been extensively studied from both experimental and theoretical points of view. Compared with their bulk counterparts, nanostructured semiconductor oxides retain rich morphologies and unusual physical and chemical properties, due to which they have wide potential applications in nanoscale devices. Tin oxide (SnO_2) has been widely studied as an n-type semiconductor; it has a band gap energy of 3.6 eV at room temperature and has been used as a promising material for gas sensors and optoelectronic devices, and as a negative electrode for lithium batteries. Therefore in the present research Tin oxide (SnO_2) nanoparticles have been synthesized by solution combustion synthesis, hydroxide method and hydrothermal route and the effect of different nanostructures and sizes on gas sensing behavior has been studied for toluene gas. Most of the VOCs are hazardous and are known to cause several kinds of diseases like allergies, asthma, cancer and emphysema. Toluene is one of the VOCs. Obtained ultrafine nanoparticles have BET surface area ~41 m^2/gm. Synthesized particles have particle size in the range of 8-20 nm. The degree of agglomeration of SnO_2 nanoparticles is calculated. The nitrogen adsorption-desorption isotherms of the nanoparticles were recorded at 77K.

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Metal oxide nanomaterials for healthcare applications

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Very recent advances in the nanochemistry and nanomaterials research has provided a new set of research tools, materials, structures and systems, for biological and medical research and applications. Thus, there has been extensive research and developments on nanomaterials for healthcare applications viz diagnostics, devices, therapeutics etc. Through the present talk, synthesis and functionalization of nanomaterials for healthcare application will be discussed. Looking at the scope of the topic, the presentation will be limited to only metal oxide nanomaterials, typically Fe_3O_4 and ZnO nanoparticles, for cancer and diabetes therapeutics. The first part will be on Fe_3O_4 nanoparticle for cancer therapeutics. Fe_3O_4 nanoparticles have been explored for a very long time as a promising drug delivery, MRI and cancer hyperthermia agent in medical diagnostics and therapeutics segment. On the other hand, curcumin, a natural organic material, due to its inflammatory suppressing, antioxidant and tumor-resistant and other such properties, is also known as 'goldmine in medicine'. But the limited bio-solubility of curcumin has restricted its widespread application. In this context, we have worked on exploring possible applications of the synthesized Fe_3O_4-curcumin conjugates using citrate linker (Fe-CA-CU), at an in-vitro level. The conjugation chemistry, the loading percentage of curcumin in the system, and the magnetic properties will be discussed. This will be followed by the in-vitro studies, indicating its potential applications in cancer therapeutics via 1) magnetic hyperthermia- site specific tumor suppression and 2) exploring the therapeutic uses (anti-oxidant and anti-inflammatory) of curcumin. The development of promising solutions in diabetes therapeutics has been another challenge in healthcare domain. The ever-increasing number of patients and the side-effects, rather adverse effects of the conventional systems-which include enzyme inhibitor, have invited many scientists to develop promising contender with minimal side-effects. As is well known, Zinc has strong role in insulin synthesis, storage and secretion and thus its deficiency can be related to diabetes. In this context, natural extract of Red Sandalwood (RSW) as a potent anti-diabetic agent, in conjugation with ZnO nanoparticles was explored. ZnO nanoparticles have been synthesized via soft chemistry routes and duly characterized. The conjugation chemistry, extract loading percentage was also studied. The anti-diabetic activity was assessed with the help of like α-amylase and α-glucosidase inhibition assay with murine pancreatic and small intestinal extracts. The results will be discussed in the presentation. Besides, the use of ZnO nanoparticle modified optical fiber sensors will be discussed at the end.

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