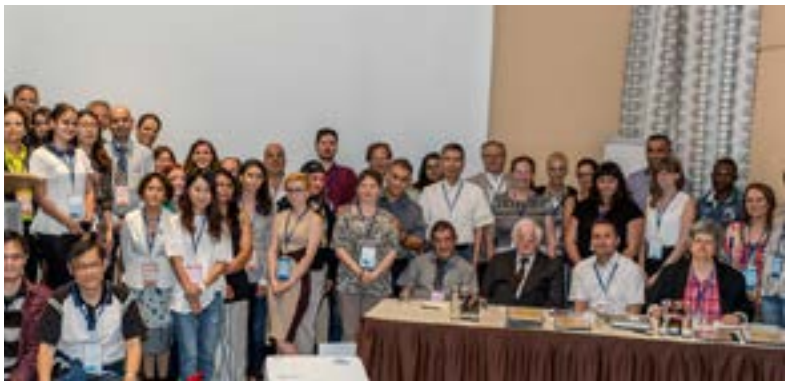
2308th Conference

Materials Science & Crystallography 2018



15th International Conference and Exhibition on

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November 07-08, 2018 | Atlanta, USA

Poster Presentations

15th International Conference and Exhibition on
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APPLIED CRYSTALLOGRAPHY November 07-08, 2018 | Atlanta, USA

Fabricating superhydrophobic surfaces for self-cleaning applications by two-step simple spray coating process

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Superhydrophobic surfaces have recently attracted a lot of attention due to their high water repellency along with a wide range of applications in many fields. The application of such surfaces for self-cleaning purposes, such as in solar cell modules, has been limited due to the lack of mechanical robustness, thermal stability and ultraviolet radiation resistance. The fabrication of superhydrophobic water-repellent surfaces with mechanical robustness and high transmittance remains a major challenge. The focus of this work is to prepare highly transparent water-repellent surfaces with improved mechanical stability/robustness by simple spray coating process. The developed coating solution can be sprayed on all kinds of materials surfaces to create a superhydrophobic self-cleaning surfaces. Proper molar ratios of Methyltrimethoxysilane (MTMS) and (3-Glycidyloxypropyl) trimethoxysilane (GLYMO) are used to bond the functionalized silica nanoparticles to various substrates and promote robustness. Optimum spraying cycles (layers) of 1.0%wt SiO_2 nanoparticles after adhesive layer has resulted in contact angles of the order of 170° with a hysteresis of 6° and sliding angle of 1°. Developed surfaces also exhibited excellent stability under simulated outdoor conditions, such as pressurized jet water, abrasion and ultraviolet radiations etc. Improvement of surface transmittance was achieved by annealing the surface under temperatures up to 300°C without losing superhydrophobicity. The optical transmittance of the optimum annealed surface varied between 75% of that of virgin glass, at the visible light wavelength of 400nm and 90% at 800nm. The developed surface during this research makes them a promising candidate for outdoor self-cleaning applications even under harsh environmental conditions.

Biography

Abuduliken Bake has completed his Bachelor's degree in Polymer Materials and Engineering from Beijing Technology and Business University in 2013. After one year of work in food processing company, he joined King Fahd University of Petroleum and Minerals (KFUPM) for Master degree in 2014. He is currently pursuing his PhD in Mechanical Engineering at KFUPM.

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Modelling and simulation sensors of mems based pressure for industrial applications

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This paper presents investigations on improvement sensitivity of MEMS-based pressure sensor for various industrial and environmental applications. It provides an overview of the design, modeling and simulation of MEMS pressure sensor. An attempt has been made to achieve high sensitivity i.e. providing different structures for membrane (circular, square, rectangle) with uniform surface area and thickness have been modeled and simulated for various loads ranging from 0.1 to 1MPa with three different materials. From the analysis of simulation results, it has been observed that the pressure sensor with circular membrane provided with aluminium material found to exhibit more deformation and high sensitivity of 28.2×10^{-6} for 10μm thickness and 45.6×10^{-6} for 7μm thickness. The reasons for enhancement in the sensitivity discussed in detail as a function of input load, geometry changes and materials addition. The software tool COMSOL Multiphysics version 4.2 is used to model the proposed design of pressure sensor. These studies are highly useful to check and compute pressure in various environmental conditions.

Biography

Vemireddy Hanumakoti graduated from Department of Electronics and Instrumentation Engineering at Lakireddy Bali Reddy Autonomous Engineering College. She is working as a Technician in the Department of Electronics and Instrumentation Engineering in National MEMS Design Centre (NMDC) since five years. She is involving and clarifying the doubts that are coming to NMDC for design and simulation by using software tool COMSOL Multiphysics. She is actively participating in department organizing conferences, workshops and seminars related to NMDC.

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A numerical analysis of the dependence of absorbed power on the size of ZnO/Au nanorod in ZnO/Au (Nanorod)-PbS (Quantum Dot) hybrid structure

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A hybrid structure of ZnO/Au core-shell nanorod (NR) on top of PbS quantum dot (QD) array is simulated for the power analysis of ZnO/Au nanorods' size dependence of absorbed power using FDTD simulator. Total Absorbed Power (TAP) is observed which is dependent on nanorod's length and radius. The radius of the ZnO/Au core-shell nanorod is 6.5nm where the ZnO core has a radius and length of 4.5nm and 38nm, respectively. The Au shell has a thickness of 2nm. As the number of NR is increased, the peak value of the total absorbed power also increases for a wavelength of 640nm. The peak value of total absorbed power for 1 nanorod and 5 nanorods is found to be 0.0366 and 0.1645 respectively. With the increase of the radius of the NR from 6.5nm to 7nm, the peak of the wavelength shifts from 640nm to 533nm. The relationship between absorbed power and wavelength is illustrated for an increasing number of nanorods.

Biography

Kanij Mehtanin Khabir has completed her undergraduate (BSc) in Electrical and Electronic department from University of Dhaka and now she is doing her graduate (MSc) in the same department. Her research interest is on nanotechnology. She has published two journals. Now she is holding position as Chair of IEEE Student Branch, University of Dhaka.

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Notes:

Ryan Sumner, Res. Rev. J Mat. Sci. 2018, Volume 6
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Rugged nanoparticle tracers for mass tracking in explosive events

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Tracing the flow of solid matter during an explosion requires a rugged tag that can be measured by a unique, identifiable signature. Small semiconductors coined "Quantum Dots" provide a unique tunable photoluminescent signature that can be tuned by the material's composition and core/shell thickness. The particles can be ruggedized by the growth of a silica surface around the quantum dots (QDs) that acts as a sacrificial layer during finite periods of elevated temperatures and pressures. Incorporating the QDs into a matrix allows for identification of the debris by its' unique photoluminescence. Five different types of zinc sulfide QDs were synthesized and encapsulated in silica shells. The silica shelled QDs were covalently bound to an inexpensive commercially available luminescent powder. The combination of 5 dots and 5 powders enables a matrix of 25 unique pigments that fluoresce at different excitations wavelengths. These pigments can be applied for mass tracking and model confirmation. The use of a commercial luminescent powder with the QDs allows for field identification and laboratory confirmation. The QD bound powders were suspended in a hydrated silica gel pending incorporation into temperature resistant paints, synthetic stone and controlled porous glass. The incorporation of temperature resistant QD bound powders has enabled unique identifiers, which allows for the tracking of mass through explosive events and other inaccessible environments.

Biography

Ryan Sumner has completed his MSc and BS in Chemistry from Western Washington University. He is currently a staff materials/analytical Scientist at Pacific Northwest National Laboratory focusing on nanomaterial fabrication/integration, method development and instrumentation. He has papers related to nanomaterial integration for renewable energies. Current research includes studies on nanoparticles for mass tracking, isolation of individual isotopes via mass-spec and development of radiochemical separations.

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Diane Moon, Res. Rev. J Mat. Sci. 2018, Volume 6
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Efficiency enhancement of anaerobic digester in microbial fuel cell through use of *R. albus*

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The current study has been undertaken to examine the beneficial effect in the power output of a microbial fuel cell (MFC) by adding cellulolytic bacteria *Ruminococcus albus (R. albus)* into the anodic chamber. Mediator-less H-type MFCs were set up where the anode chamber contained anaerobic digester microorganisms as inocula on the finely ground pine tree (Avicel) at 2% (w/v) and the cathode chamber of 10mM phosphate buffered saline conductive solution, both separated by a cation exchange membrane. The functioning of the MFCs for generation of electrical power and the amounts of gaseous byproducts was monitored over a 9 day period. The addition of cellulolytic bacteria caused an increase in average power density from 7.9mW/m^2 to 19.5mW/m^2, about 245% increase over a 9 day period. For both groups of MFCs; with *R. albus* and the control, the headspace gases collected were methane and CO_2. While the methane: CO_2 ratios were found unchanged at 1.7:1 throughout the 9 days of observation, the total gas production increased from 248mL to 319mL due to the presence of *R. albus* addition. This study confirms that whereas the biocatalytic activity of anode microbial population determines the energy production, the addition of external cellulolytic bacteria into anode microbial population can improve and extend the biomass utilization.

Biography

Diane Moon is a student of The Gwinnett School of Mathematics, Science and Technology, Lawrenceville, GA. She worked with Dr Paul S Chung in Fuzbien Technology Institute. Her research field was green energy and her research results have been published in the journal.

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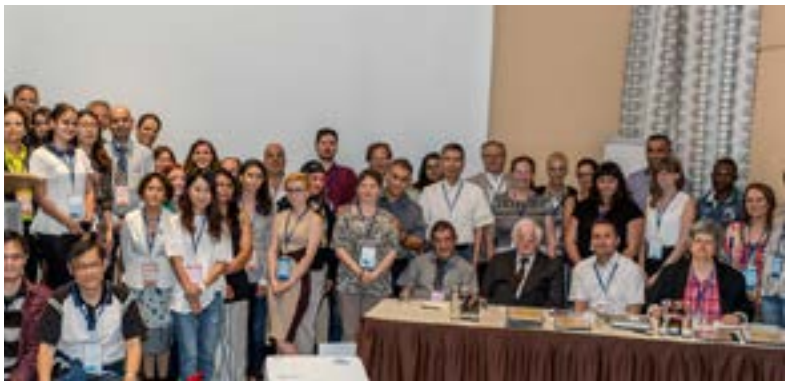

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Designing and probing ultrafast energy/charge transfer kinetics in Ruddlesden-Popper perovskites and QDs attached photochromic devices

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The semiconductor perovskites materials and quantum dots (QDs) demonstrate outstanding optical properties. The perovskites exhibit wide color emission that makes them the highly suitable candidate for LEDs and QDs exhibit narrow emission that makes them suitable for fluorescent probes. 2D organolead halide perovskites and their 3D analogous have exhibited encouraging performance metrics of LED, like low turn-on voltages and external quantum efficiencies. An optical cascading mechanism is observed in electrically emissive Ruddlesden-Popper (RP) perovskite series ($(C_8H_{17}NH_3)_2(CH(NH_2)_2)_{m-1}Pb_mBr_{3m+1}$). A mixture of 3D formamidinium lead bromide $CH(NH_2)_2PbBr_3$ and 2D octyl ammonium lead bromide $(C_8H_{17}NH_3)_2PbBr_4$ perovskite (~0-80% 2D) are prepared to develop an understanding regarding the energy cascading mechanism. Ultrafast transient absorption and fluorescence techniques suggest energy transfer from high bandgap "donor" too low bandgap "acceptor" in RP perovskite films for 20% (2D) mixed RP perovskite. Following excitation at 400nm in RP very fast decay of 435nm exciton and very fast rise (390 ft) of 535nm bleaching signal suggest very efficient energy transfer from donor to acceptor for 20% 2D perovskite. By further increasing the concentration of 2D in 3D RP perovskites, energy transfer is delayed and it deteriorates the LED efficiency due to incomplete energy transfer. These findings shed light on the importance of engineering the acceptor to donor ratio to gain efficient energy transfer. Parallelly in II-VI semiconductor QDs attached photochromic azobenzene molecules a fast charge/energy transfer is observed. Upon UV irradiation, the photoresponsive azobenzene undergoes a reversible trans-cis isomerization. The photoinduced trans-cis transformation helps to transfer photoexcited charge/energy transfer from the conduction band of the QDs to the LUMO of the cis-isomer of the azobenzene. As a result, the fluorescence of QDs can be modulated to fabricate fluorescent probes for a wide range of optical applications.

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Structural changes in lead phosphate glasses doped with vanadyl

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A series of lead phosphate glasses doped with vanadyl were prepared by a single-step process from PbO and $NH_4H_2PO_4$. In these glasses, the transition metal ion as vanadyl VO^{2+} ion derived from $VOSO_4 5H_2O$ as VO^{2+} (VS) doped and VO^{2+}(VP) is used as another dopant derived from V_2O_5. A Thorough Knowledge of optical properties of transparent glasses will enable successful utilization of glasses for optical applications such as windows, filters and lasers. The optical absorption spectra of these glasses in the ultra-violet region have been recorded. The results obtained on the electronic absorption spectra observed to d-d bands. The VO^{2+} ions along with the double-bonded oxygen exist in a molecular complex which is identified as VO_5 polyhedra in lead phosphate glass network. As the PbO content in the glass increases, structural changes take place in the network. The IR spectra of these glasses were also presented with the results. The glass-modifying role of PbO is extendable up to 66.6 mole% with the glass former P_2O_5. The differences in the IR spectra of phosphate glasses of various compositions arise presumably from the chains being polymerized to different extents. The role of PbO as glass modifier is almost quantitatively determined by the amount of P_2O_5. The characteristic IR band due to the P=O bond in the P_2O_5 network is retained until the composition of pyro-phosphate quenched samples (x=0.66) suggests that PbO does not act as a "glass former" and no complete rupture of the glassy network by Pb^{2+} takes place.

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Challenges of the inverse problem of the diffraction X-ray Topo-tomography: Theory, formulas and computer iterative algorithms towards the 3D reconstruction of elastic statical displacement field around the point-defects in a crystal

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In the recent 10 years, the Diffraction X-ray Topo-Tomography (DXTT) is widely applied to the structural analysis of real crystals. In the DXTT method the crystal plate is rotated around an axis perpendicular to the reflecting planes net, usually the rotation axis 0X is selected along the diffraction vector h. Then, the 2D-projection set (the diffraction X-ray image topograms-DXITs) is collected for different rotation (inclination) angles Φ, each of which is related to some inclination of the diffraction X-ray plane with respect to the intrinsic coordinate system of the crystal sample, the axis 0S is along the wave vector kh of the diffracted wave propagation. An idea of the computer restoration of the spatial defect positions in a crystal and, what is more important, the local 3D static displacement fields around defects in crystalline materials according to the DXTT data is of a special interest. such a problem is equally, if not more, directly related to the quantitative interpretation of defect imaging on the DXITs. The latter is due to the different defect imaging mechanisms in the near and far regions surrounding the crystal lattice defects. In the present report, the semi-kinematic analytical solution of the dynamical Takagi-Taupin equations for the diffracted wave amplitude Eh(r) is built that allows in general to develop the consequent theoretical approach for resolving the inverse DXTT problem. As an example, using the one 2D projection data with inclination angles Φ=0, the results of the computer restoration of the 3D displacement field function $f(r-r^0)=h\cdot u(r-r^0)$ around the Coulomb-type point defect in crystal Si(111) are reported and discussed (diffraction vector h=[2 ¯22], the X-ray MoKα1-radiation, the wavelength λ=0.071nm, the Bragg angle θB=10,65°. $u(r-r^0)$ is the near field of elastic static displacements around the Coulomb-type point defect at the point r^0). Respectively, to computer restoration of the 3D displacement field function $f(r-r^0)$ the simulated annealing and Quasi-Newton gradient descent algorithms are applied to our problem. To obtain a good solution convergence, some physical constraints onto the type of functions $\{f(r-r^0)\}$ searched are imposed. The 2D numerically simulated and then, used for the computer 3D restoration of the theoretical function $f(r-r^0)$ is by using the Quasi-Newton descent algorithm, the cross-section pictures of the theoretical function $f(r-r^0)$ and the ones restored from the 2D projection in planes z=const. z(dimensionless units)=(A) 6, (B) 8, (C) 10, in are depicted The case (B) is related to the mid-thickness of Si(111) plate.

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Synthetic phase and morphology control over colloidal nickel sulfide nanocrystals

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Binary nickel sulfides exist in a variety of phases and stoichiometries, including NiS_2, Ni_3S_4, α-NiS, β-NiS, Ni_9S_8, Ni_7S_6 and Ni_3S_2. Distinct phases of the binary nickel sulfide system have potential to be used as bifunctional catalysts for water splitting, cathode materials for lithium-ion batteries, absorber layers for solar cells, hydrodesulfurization catalysts, or supercapacitors. However, the complicated nature of the Ni–S phase diagram makes the solution synthesis of phase-pure colloidal nanocrystals challenging. In this presentation, the phase- and morphology-controlled solution synthesis of colloidal nickel sulfide nanocrystals is demonstrated. Nanocrystals of Ni_3S_4, α-NiS, β-NiS, Ni_9S_8 and Ni_3S_2 can be independently prepared by tuning key synthetic parameters of S:Ni precursor ratio, capping ligand, reaction time and temperature. S:Ni ratio and temperature influences the phase of nanocrystals, a phase transformation from cubic Ni_3S_4 to hexagonal α-NiS and then rhombohedral β-NiS with increasing S:Ni ratios and temperature is observed. 1-dodecanethiol is shown as an important phase and shape-directing agent. In the presence of 1-dodecanethiol, Ni_9S_8 nanocrystals with quasi-spherical morphology or Ni_3S_2 nanoparticles with a multi-pod like morphology can be obtained by using various disubstituted thioureas are sulfur precursors.

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Understanding the mechanism of indomethacin-saccharin co-crystal formation using in-line monitoring system with focused beam reflectance measurement and particle vision measurement

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The co-crystal approach has attracted enormous attention in attempts to improve critical pharmaceutical attributes such as the solubility and stability of drug substances. In 2016, the US FDA reclassified the pharmaceutical co-crystals as a special case of solvates and hydrates where the second component, the coformer, is nonvolatile, modifying their earlier viewpoint as a drug product intermediate (DPI) or as an in-process material in 2013. In the 2016 guidance, the FDA describes: "co-crystals can be tailored to enhance drug product bioavailability and stability and to enhance the processability of APIs during drug product manufacture". In-line monitoring technology is not only a significant tool for processes with high risk such as crystallization but also conforming to the global quality systems for pharmaceutical products. In this study, we attempted to clarify the formation of transient Indomethacin (IMC) meta-stable form as well as Indomethacin-Saccharin (SAC) co-crystal particles with the addition rate of anti-solvent as critical process parameter and in-line monitoring tools. Among various in-line monitoring instruments, we employed FBRM (focused beam reflectance measurement) and PVM (particle vision measurement). The characterization of in-process and post-process particles was performed via PXRD (powder X-ray diffraction) and DSC (differential scanning calorimeter). It was observed that the pathway to the final IMC-SAC co-crystal was greatly affected by the anti-solvent addition rate and process conditions to obtain high-quality co-crystal powder effectively were established. Accordingly, it is concluded that in-line monitoring based on FBRM and PVM can be a very useful PAT tool for QbD implementation.

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Crystallographic searches for weak interactions: The limitations of data mining

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The oldest and most successful application of data mining in chemistry is without a doubt the use of crystallographic databases. The common practice is to draw conclusions from the frequency of contacts observed in crystals to the relevance of the underlying non-covalent interactions. While this strategy has provided a wealth of information on structural data for stronger interactions it can be misleading in the search of weak interactions. This is illustrated by controversies about the hydrogen bond acceptor quality of organic fluorine, which culminated in the statement by Dunitz *et al.*, that "Organic Fluorine Hardly Ever Accepts Hydrogen Bonds", based on their finding of only 0.6% relevant hits in the CSD. The problem is that weak acceptors such as fluorine are introduced in thousands of compounds for very different reasons and then rarely can compete with other non-covalent interactions which can dominate in a given structure. Proposals to limit such situations in crystallographic searches will be presented, including complementary methods to measure related interaction energies in solution.

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Engaging undergraduate researchers in macromolecular crystallography

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Ground-breaking work in bringing sophisticated X-ray diffraction methods within the reach of undergraduate researchers has been reported by established leaders in the field. The Department of Chemistry and Biochemistry at California State University is committed to providing undergraduate students opportunities to engage in independent, state of the art and cutting-edge research through its capstone CHEM 495 course. Since crystallographic structure determination is the mainstream technique and plays an ever-increasing role in pharmaceutical and biotechnology strategies, we sought to bring opportunities for undergraduate researchers to embrace X-ray diffraction methods and three-dimensional structure determination for improving an understanding of structure and function in for their projects. However, this method requires a significant investment in equipment and computational infrastructure which are inaccessible to most undergraduate programs. Fortunately, resources have been made generously available to us in Fullerton through the Stanford Synchrotron Radiation Lightsource and the UCLA-DOE Institute for Genomics and Proteomics. At these facilities, undergraduates have access to high-throughput crystallization robots and synchrotrons to collect X-ray diffraction data. Utilization of these resources has created unique opportunities for teams of undergraduate researchers to tackle novel research projects including the structure determination of ADP-Glucose Pyrophosphorylase (ADPG-PPase) a key enzyme involved in rate-limiting step of starch synthesis the from the thermophilic marine bacterium *Thermotoga maritima* and a key protein designated Orf19 that believed to catalyze one of the steps in the synthesis of tetrahydromethanopterin (THMPT). In several species of archaeal microbes that live in the digestive tract of ruminants including cattle, THMPT is a cofactor that is required for the production of methane. Methane is a potent greenhouse gas; therefore inhibition of the enzymes involved in THMPT biosynthesis is a promising strategy to help mitigate the emission of this gas from large-scale cattle and dairy farming. Knowledge of the structure of Orf19 is likely to lead to a better understanding of how effective inhibitors of the enzyme can be designed for diminishing the production of methane.

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Influence of patterned substrates on miniaturization of surface patterns in soft elastic films

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The advantages of diminutive-size surface-patterns have been harnessed by various industries, such as semiconductor, integrated circuits, nano-devices, nano-sensors, optoelectronics etc. Patterning the soft thin elastic films through self-organization is found to be a cheaper alternative route for fabricating meso/nano length scales at such soft interfaces compared to conventional lithographic techniques. Self-organization involves surface reorganization of a polymeric film resting on a substrate, due to the application of a force field created by an external contactor. The film reorganizes itself to attain the minimum energy state that leads to the surface-patterning. For elastic thin films cast on smooth substrates, the instability length scales between the contact zones have been reported to be ~2.96*h (h being the mean thickness of the elastic film). Linear stability analysis and numerical simulation studies on soft elastic thin films show that much smaller pattern length scales can be obtained for sinusoidal-patterned-substrates when used in lieu of flat substrates. Inspired by the theoretical work, we have performed soft film adhesive experiments on three patterned substrates created from naturally occurring water lily leaves, low-cost commercially available compact disks and EBM created cubic patterns. The morphological surface patterns of columns, labyrinths and cavities formed at different stages of the adhesion-debonding cycle in these experiments do indeed reveal minuscule length scale formation that is much less than 2.96*h. Thus, the present work experimentally and through numerical simulations demonstrates a simple and uncomplicated method to create miniaturized patterns, which have extensive applications in fabricating lab-on-chip devices, self-cleaning materials, scaffolds for tissue engineering etc.

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Self-assembly of organic chromophore nanostructures

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The supramolecular arrangement of porphyrins and other organic molecules has great potential in the fields of molecular information storage and sensing due to their ease of deposition and good chemical and thermal stabilities. In particular, porphyrins of relatively large molecular weights can be applied in thermal deposition while tetrapyrrole molecules have had an extensive synthetic chemistry developed, which enables synthesis of complex derivatives. In this work, we present complementary examples of porphyrin nanoarchitectonics. Starting from simple symmetrical phenol derivatives, we describe the effects of steric hindrance about the respective hydroxyl groups and also the effects of conformational variation on the self-assembly structures. We also investigated fabrication of binary molecular monolayers using two different porphyrin molecules *tetrakis*(3,5-di-t-butyl-4-hydroxyphenyl)porphyrin and *tetrakis*(4-pyridyl)porphyrin by deposition in ultrahigh vacuum. This leads to two unusual heteromolecular monolayer structures were observed with one exhibiting good separation of molecules within the monolayer. Meanwhile, a synthetic nanoarchitectonic approach was used to prepare self-assembled molecular nanowires at a mica substrate. The nanowires could be observed growing using atomic force microscopy (AFM) and the network structures of the nanowires can be influenced by manipulation using the AFM probe tip. Formation of molecular monolayers with chromophores positioned remote from the substrate surface will also be discussed.

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Etching rate reactions on titanium surfaces under various electromagnetic radiation frequencies

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The surface topography of medical implants is critical to their successful integration in the human body. To ensure optimum bone-apposition, the surface of the implant material (e.g. titanium) should be modified to include desirable micro-, sub-micro- and nano-topography features, multiscale features. This research outlines critical background information to understand the importance of surface topography features on osseointegration. It also details experimental findings on the etching rate of sulfuric acid (H_2SO_4) on titanium coupons. Once the reaction rate of sulfuric acid and titanium was understood at various temperatures and time periods, it was necessary to find a mechanism to control the reaction rate. The report suggests the use of electromagnetic radiation (EMR) to control the reaction rate and outlines the experimental findings of preliminary tests between titanium and sulfuric acid under the presence of EMR. This report describes attempts to develop and realize replicate of rough surfaces containing multiscale features.

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A century after the Braggs on precision and accuracy of single crystal X-ray results

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So far, more than 1.4 mln organic, inorganic and macromolecular structures have been solved and refined by single crystal X-ray analysis. It is incredible that the Independent Atom Model (IAM) of electron density, effectively introduced a century ago, is still the most common model used in structural analysis. Its success has dominated the whole field of X-ray diffraction for the past century and for years now plays, quite a negative role. When IAM was introduced, Max von Laue, the Braggs, were using home-made pieces of equipment which could have hardly supplied any qualitative information on diffraction spots. In consequence, the errors associated with the model of electron density were overshadowed by far larger diffraction hardware errors. However, within the past century, there has been an overwhelming progress in the design and production of X-ray hardware made for the needs of both small laboratories and large-scale facilities. This progress should also accelerate progress in the quality and complexity of models of electron density used to interpret experimental results. I will discuss the precision and accuracy of single crystal X-ray results obtained for multiple measurements of single crystals of oxalic acid as a function of the resolution of X-ray data and the quality of electron density model applied (IAM, multipole model (MM), Hirshfeld Atom Refinement (HAR) and Transferable Aspherical Atom Model of electron density (TAAM)). I will present a detailed comparison of structural, thermal and electronic parameters obtained for the same multiple diffraction data sets collected for single crystals of oxalic acid when different models of electron density are refined. Practical suggestions will be presented how to estimate and improve the quality of structural results. Among others with the newer models, one can obtain more precise and accurate information on positions of H-atoms or energy of intermolecular interactions in crystals.

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The Berkeley Center for structural biology suite of crystallography beamlines at the advanced light source

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Structural biology continues to revolutionize the way we understand life sciences at a molecular level. Critical to structural biology is macromolecular crystallography and the absolute requirement of acquiring X-ray diffraction data from increasingly challenging samples. The Berkeley Center for Structural Biology (BCSB) brings 20 years of experience to beamline management and innovation. We operate five high-throughput protein crystallography beamlines at the Advanced Light Source at Lawrence Berkeley National Laboratory and are complementing our portfolio with the addition of a new microfocus beamline. Our vision is to provide state-of-the-art beamlines through continual development and outstanding service for crystallographers around the world, enabling structure solution on even the most complex biological systems. BCSB innovations include the pioneering of the automatic robotic sample changer, the development of a compact variable collimator to define the size of the beam and the measurement of the sample flux through a compact diode beam stop. To facilitate the beamline experience a graphical user-friendly interface was developed and over the years refined and streamlined to fit the needs of the crystallographers. The majority of the BCSB users are now shipping their samples and using the beamlines remotely from their home institutions. In recent years a series of new tools were implemented taking advantage of BCSB innovations and fast-framing detectors. Now crystallographers can use a queuing approach to speed-up sample screening, diffraction-based raster search to locate micron-size crystals in a sample and vector/helical data collection to minimize radiation damage. In the last year, we have implemented a user-free automatic approach for sample screening and full data collection. Quite often the automated approach identifies good quality data from samples that would otherwise have been missed. The automatic data collection approach has proven valuable to fragment-based screening and drug design. Together with the automatic processing of datasets, users can focus on structural biology rather than details of data collection.

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Nanocellulose: The next generation of super materials

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Cellulose is one of the most abundant natural resources on this earth and it is one of the most important structural components of the primary cell wall of green plants, many forms of algae and the oomycetes. Cellulose history dates back to as early as the 1860s when the first rayon fibers were commercialized by Courtaulds. Although cellulose has a long history in the commercial market, its incompatibility with most polymer matrices, tedious extraction processing and large amounts of energy and time needed to extract and convert to nano cellulose form has lessened its attractiveness for use in the design of bio-based materials. That being said, our group research has focused on the extraction and modification of micro- and nano cellulose and its dispersion into biodegradable and non-biodegradable polymer matrices to form bio-based plastic materials. This presentation will report on our investigation of the influence of cellulose micro fibrils and nano fibrils, CMFs and CNFs, respectively, dispersion on the thermal, mechanical and biodegradable properties of polymeric composites. In summary, our research has observed an increase in the thermal stability of modified CMFs and CNFs when compared to their unmodified cellulose counterparts. Dynamic mechanical analysis(DMA), thermal mechanical analysis (TMA), show marked improvements in the mechanical properties of the cellulose-based composites when compared back to its neat counterpart.

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Preparation and characterization of X-ray mirrors and development of thin-film metamaterials for thermal photovoltaics

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Magnetron sputtering is a versatile tool to synthesize nanocrystalline or amorphous phases with well-adapted material properties. This thin-film method enables us to coat very precisely, uniform and flexible. High surface quality is required in a variety of technical applications, such as architectural glass, metallic surfaces and especially for X-ray mirrors. Another advantage is that it is applicable to materials with a very high melting point, which opens the use of refractory metals. This presentation will focus on two research fields, which exploit the mentioned advantages for thin-film preparation of X-ray mirrors and thermophotovoltaic metamaterials. Large X-ray mirrors are required for beam transport at free-electron lasers (FELs) and synchrotron sources worldwide. The demand for large mirrors with lengths up to 1m single layers and multilayers consisting of light or heavy elements has increased during the last few decades. At the Helmholtz-Zentrum Geesthacht (HZG), a 4.5m-long sputtering facility enables us to deposit a desired single-layer material some tens of nanometers thick. For the European XFEL project, the shape error should be less than 2nm over the whole 1m X-ray mirror length to ensure the safe and efficient delivery of X-ray beams to the scientific instruments. The challenge is to achieve thin-film deposition without any change in mirror shape. Magnetron-sputtered thermophotovoltaic metamaterials are synthesized to obtain a selective thermal emitter. We demonstrated the high-temperature stability of W/HfO_2 metamaterials till 1000°C. The experimental results achieved will be discussed with regard to current restrictions and future developments.

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Preparation and properties of the water-soluble copolymer and applied in bioimaging

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Near-infrared absorption materials have shown great application prospect in the fields of biology, energy and materials industry. However, water-soluble polymer composites with near infrared absorption, high thermal stability and well film-forming properly have rarely been reported. In this work, the novel polyacrylamide composites with near infrared absorption were designed and prepared. Our system solves the problems of water solubility, toxicity and the inability to target specific tissues exist in the traditional materials used in cancer cells application (cellular imaging) in past years ago and our structure, composition, properties were characterized and evaluated by ^{1}HNMR spectrum, ^{29}Si NMR, Fourier transform infra-red spectroscopy (FTIR), DSC, TGA, UV-Vis-NIR, GPC and Fluorescence spectra properties. It was found that the resultant hybrids possess have no cytotoxicity, soluble in water immediately, good permeability and high photostability in living cells and has been applied successfully.

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Large-scale growth of lead iodide hydroxide microwire crystal for an X-ray detector

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Very recently, lots of efforts focused on one dimensional (1D) laurionite-type lead halide hydroxide Pb(OH)X (X=Cl, Br, I) due to their extraordinary structural and spectral characteristics. In this paper, we report a successful facile growth of freestanding lead iodide hydroxide (Pb(OH)I) microwire crystal via hydrothermal method without additives. The properties of the samples were investigated by SEM, EDS and single crystal X-ray diffraction. The results show that Pb(OH)I microwire crystal is an indirect band gap semiconductor material (2.823eV) based on density functional theory (DFT). Moreover, the Pb(OH)I microwire crystal based photodetector respond to x-ray incident light with a fast, repeatable and stable response characterized by a reasonable response and decay times (0.13s and 0.29s, respectively). These results substantiate the potential of Pb(OH)I microwire crystal as a candidate material in optoelectronic applications.

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Strongly circularly polarized luminescence from dinuclear Eu(III) helicates prepared through a BINOL-based bis-β-diketone ligands

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Chiral lanthanide helicates have potential applications in biology and material science as chiral probes and circularly polarized luminescence (CPL) materials. However, the preparation of homochiral helicates through coordination-directed self-assembly strategy is challenging due to the greatly labile coordination geometries of lanthanides, which raised the higher requirement for ligand designs. Herein, a BINOL-based bis-β-diketone ligand is developed, which give rise to preorganized helical conformation and induced the formation of homochiral helical structure. X-ray crystallographic analysis reveals that the ligand assemble with Ln(III) ions to give homochiral either P or M quadruple- and triple-stranded helicates, [HNEt3]2+•[Eu_2(BTTB)$_4$]2- and Eu_2(BTTB)3(R/S-BINAPO)2 {(R/S)-BINAPO=(R/S)-2,2'-bis(diphenylphosphoryl)-1,1'-binaphthyl; BTTB=bis[4-(4,4,4-trifluoro-1,3-dioxobutyl)(2,3,5,6-tetrafluorophenoxyl)]-1,1'-binaphthalene}. The ^{1}H, ^{31}P NMR and CD measurements confirm the diastereo purity of the assemblies in solution. A detailed optical and chiroptical characterization reveals that the luminescent enantiopure helicates not only exhibit intense circularly polarized luminescence (CPL) with |glum| values reaching 0.80 but also show high luminescence quantum yields of 72.8%. Our results provide a feasible strategy for designing homochiral helical lanthanide supramolecular architecture and synthesizing excellent CPL materials.

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Study on uniaxial tensile and creep deformation of structural steel

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Creep resistant Ferritic-Martensitic steel is considered as a promising structural material for power plant applications. For such steels, intensive research have been carried out in the scientific world to understand the high-temperature deformation mechanism both through uniaxial Constant Strain Rate Test (CSRT) and Creep test at 0.3-0.5Tm. However, very few attempts were made to correlate the effective stress of CSRT with actual creep rate. The present work is an attempt to establish a relationship between these two. To characterize the stress exponent (n) and activation energy (Q) of F92 steel, experiments were carried out via Differential Strain Rate Test (DSRT) and CSRT between strain rate range of (10^{-5}-$10^{-3}s^{-1}$) and temperatures (400-700^{0}C). The estimated (n) and (Q) through CSRT were found to be 13 and 600kJ/mol, respectively. To rationalize high obtained values of n and Q, BMD model was used and rationalized values came to be 5 and 236±20kJ/mol, respectively. The values of n and Q were also obtained directly from DSRT and found to be 4±0.2 and 195±2kJ/mol, respectively, which are close to the values obtained from CSRT. These values reported being associated with the climb of edge dislocation deformation mechanism. The CSRT results were further analyzed for identified n≈4-6 to predict steady-state creep rate (ɛ̇ss) for corresponding effective stress (σ-σ^{th}) which is reported to be responsible stress for creep deformation and further validated by conducting creep test. Microstructural characterization of the samples was carried out under TEM and the metallurgical factors identified affecting the results.

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Microstructural evolution of nanocrystalline tungsten-25% rhenium-hafnium carbide composite synthesized by spark plasma sintering technique for FSW tool application

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Development of nanocrystalline tungsten-25% rhenium alloy reinforced with hafnium carbide is a challenging task as these alloys are difficult to synthesize by conventional methods. The problem of these difficult to alloy elements can be addressed by using a unique combination of mechanical alloying and spark plasma sintering (SPS) techniques via powder metallurgy route. Rhenium was added to a lower ductile-to-brittle transition temperature and to increase recrystallization temperature of tungsten. SPS is a rapid consolidating technique which prevents grain growth. These tool materials can withstand high temperatures and harsh conditions in joining application such as Friction Stir Welding (FSW) of steel and titanium alloys. FSW is a green process which does not emit fume and toxic fumes during the process. Sintering was carried between 1500-1800°c. Mechanically alloyed and spark plasma sintered alloy and composite were characterized by optical microscopy, field emission scanning electron microscopy (FESEM) and X-ray diffraction. Microstructural investigation of consolidated specimens was initially carried out by conventional etching and metallography techniques. Optical micrographs showed no visible signs of grain boundary etching. Spark plasma sintered samples were further electrochemically etched in one molar concentrated solution of NaOH. The positive terminal of the low voltage direct current power supply was connected to the sample. The negative terminal was connected to a steel plate acting as a cathode. Both electrodes were placed in the tank face to face with a gap of 6 to 10 centimeters between them. The voltage was kept constant at 5 volts during the etching process. The sample was etched for a short time interval from 1 to 5 seconds and microstructural analysis was conducted after each etching step. The results of the FESEM images confirm microstructural revelation of these difficult to etch alloy and composites.

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