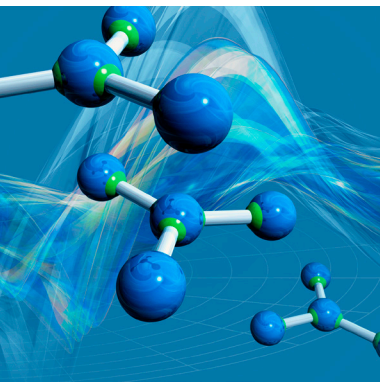
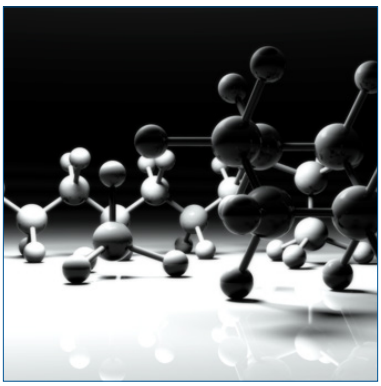
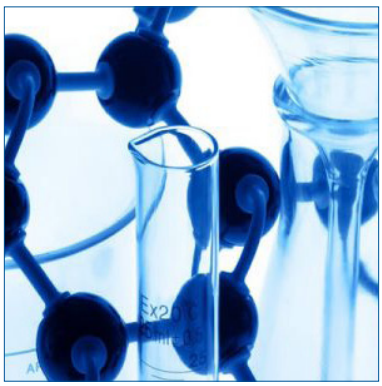
Scientific Tracks & Sessions
November 22, 2018

Materials Physics 2018



International Conference on

Materials Physics and Materials Science

November 22-23, 2018 | Paris, France

Phase transitions in $Bi_{0.5}Na_{0.5}TiO_3$ based Ferroelectrics

Yan H
Queen Mary University of London, UK

Lead-free $0.94(Bi_{0.5}Na_{0.5}TiO_3)–0.06(BaTiO_3)$ (BNTBT) is a potential piezoelectric candidate to replace lead-based PZT ceramics. The thermal depoling temperature sets the upper limit for the high temperature application of piezoelectric materials. Recently, an interface model was proposed to explain the good resistance to thermal depoling of BNTBT-ZnO composite. However, we found that the presence of ZnO was not limited to the interface but contributed intrinsically to the BNTBT lattice. This played a critical role in the structural changes of BNTBT, confirmed by a unit volume change supported by XRD, which was further proved by Raman, EDS, and dielectric characterization at different temperatures. The previous interface model is not correct because BNTBT shows thermally stable piezoelectric properties, even though there is no interface between BNTBT and ZnO. The thermal depoling behaviour of BNTBT-based materials is directly related to the transition temperature from the rhombohedral phase to the tetragonal phase in our phase transition model, which is consistent with four current peaks in their ferroelectric loops close to the depoling temperature.

Speaker Biography

Yan H is a senior lecturer in materials at the school of engineering and materials science in Queen Mary, University of London. He received his PhD in materials science and technology from Shanghai Institute of Ceramics in 2001. Since that, he joined QMUL as an academic visitor and research assistant. At QMUL, he was appointed as an academic Fellow in 2011 and senior lecturer in 2015. His research area includes: processing and analysis of the microstructures and properties of advanced materials with textured, nano and metastable structures, covering dielectrics, ferroelectrics, thermoelectrics and ceramic-CNT composites. He has over 100 publications that have been cited over 3600 times, and his publication H-index is 35 and has been serving as an editorial board member of Advance in Applied Ceramics and Materials Research Bulletin.

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Electrospinning and mechanotropic phase separation

Sergey Kotomin
Russian Academy of Sciences, Russia

Electrospinning from polymer solutions is widely used for manufacturing of nanofibrous materials. For a long time, the mechanism of electrospinning was related to fast evaporation of solvent from thin liquid jets of polymer solution in high voltage electric field. We suggest for that process another mechanism – phase separation as a result of high speed stretching typical for electrospinning. Under elongation the solution undergoes phase separation and the solvent reveals on the surface of the fiber without its complete evaporation.

Speaker Biography

Sergey Kotomin is a professor, department of chemistry, Bauman Moscow State Technical University, leading research scientist, A V Topchiev Institute of Petrochemical Synthesis, RAS. Author of 120 scientific publications in the field of physical chemistry and processing of polymers and composites.

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Can standard DFT calculations correctly describe the physical properties of AlOOH under pressure?

Cortona P
University of Paris-Saclay, France

The behaviour of AlOOH under pressure has been the object of many experimental studies. Under ambient conditions, AlOOH is stable in the α phase (also called diaspore). The δ phase becomes the stable phase at about 17 GPa, while a third phase (called γ phase or boehmite) is metastable. These three phases differ for the arrangement of the oxygen octahedra surrounding the Al atoms and for the kind of hydrogen bond connecting the octahedra.

AlOOH equations of state have been reported in various papers, but, even when the p-V data collected by different researchers agree quite well, the bulk moduli obtained by fitting the data with Birch-Murnaghan or other analytical equations of state are very different. Quite strangely, large discrepancies are also found among the theoretical results, even if the calculations have been done using the same approximations.

I will discuss the origin of these uncertainties by mean of DFT calculations. Furthermore, I will show that the use of GGA for solids (like PBEsol or TCAsol) is mandatory to obtain a satisfactory and quite accurate description of this system. I also discuss the symmetrisation of the hydrogen bond in the δ phase. There is a long-standing debate about the pressure at which the symmetrisation of the hydrogen bond takes place. I will show that PBEsol and TCAsol allow one to come to a quite convincing and well-defined conclusion.

Speaker Biography

Cortona P is professor of physics at University of Paris-Saclay, France. His research domain is mainly the density functional theory and its applications to solid-state and surface physics. Among his more recent achievements it can be mentioned the PBE0-1/3 hybrid and the TCA and SG4 GGA functionals. He was the author of the so-called density-functional theory for subsystems.

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Obtaining of graphene/polymer composites by hydrosilylation reaction for SLA printer

Natia Jalagonia
Vekua Sukhumi Institute of Physics and Technology, Georgia

Three-dimensional (3D) printing is often considered synonymous with additive manufacturing. Several types of 3D printers are known where we usually used polymers are. Stereolithography (SLA) employs a single beam laser to polymerize or crosslink a photopolymer resin. By drawing on the liquid photopolymer resin with a light beam, thin layers of polymer are stacked layer by layer. Elastomer based on polydimethysiloxanes (PDMS) are important class of materials, because of properties such as chemical inertness, flexibility, optical transparence, also they have a very low surface tension (20.4mN/m) and glass transition temperatures (146K). it is possible to print a support material that holds the PDMS prepolymer in place until it can be cured by UV light using a photoactive cross-linking agent. It is possible to graft photoactive group on PDMS backbone and obtain new UV curable polymer. The aim of presented work is obtaining of photopolymers based on PDMS. For purpose, we have conducted hydrosilylation reaction of polymethylhydrosiloxane (PMHS) with allyl acrylate and vinyltriethoxysilane in the presence Karstedt's catalyst in Toluene. Obtained polymer is liquid which are well soluble in organic solvents with specific viscosity $\eta sp \approx 0.4$. The end of reaction was tested by FTIR, where peak at 1260 cm^{-1} disappears which belongs to Si-H bonds. After this the polymer distilled in vacuum, cross-linking agent was adding about 1% and curried by UV during 1h.

Speaker Biography

Natia Jalagonia has completed her PhD at the age of 31 years from Tbilisi State University, Georgia. She is the head of Chemical Technology Laboratory of Ilia Vekua Sukhumi Institute. She has over 30 publications.

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Highly sensitive and selective gas sensor utilising tips pentacene based organic thin film transistor

Amjad Al Shawi
Bangor University, UK

Organic sensing technology has been widely investigated in the last few years. The low fabrication cost, high sensitivity, short response and recovery time allowed this type of sensors to dominate the research activities in academia and industry. In this work, solution processed organic thin film transistors (OTFTs) based on 6,13-bis (triisopropylsilylethynyl) (TIPS) pentacene were fabricated and characterized using the bottom-gate, top-contact (B-G, T-C) configuration. After preparing clean glass substrate, a 50nm aluminium was thermally evaporated as the gate electrode. The insulating layer was spin coated (2000 rpm) from a cross-linked polymethyl methacrylate (cPMMA) 5% anisole solution by using [1,6-bis(trichlorosilyl) hexane (C6-Si) (10µ/1ml) as a cross-linking agent to produce 330nm layer thick. Tips-pentacene semiconductor (2% toluene solution) was drop coasted on the cPMMA layer as the active layer. Finally, gold electrodes of 50nm thickness were thermally evaporated on the TIPS-pentacene active layer to provide the drain and source. After exposing the OTFTs to different concentrations of ethanol vapour, the current-voltage characteristics of the OTFT sensor and the response to different concentrations of ethanol (from 1ppm to 8ppm) were investigated. The output characteristics (VDS = 0 – (-60) V) with different gate voltages (VGS= 0 – (-50) V) and different ethanol concentration were investigated. It was found that the drain source current in the saturation region decreases rapidly when the OTFT was exposed to ethanol vapour at room temperature (~25 Co). Furthermore, the transfer characteristics with different ethanol concentrations showed a clear shift in the threshold voltage, which increased (from -2V to -18 V) with increasing the ethanol concentration.

Therefore, the source drain current in the TIPS pentacene based OTFTs can be considered as a significant parameter to monitor chemical species and it can be used as a sensor for chemical gases.

Speaker Biography

Amjad Al Shawi is a PhD student at the school of electronic engineering, Bangor University, UK. He is in his third year of the PhD in the field of organic transistors and organic memory devices. He completed his B.Sc and M.Sc study in physics from Basra University, Iraq. He worked as a researcher in the Polymer Research Centre at Basra University.

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Experimental and numerical investigations of the effect of nano-coatings of window glazing on thermal behavior of buildings in Saudi-Arabia

Ahmed Mohammed Almogbel
King Abdulaziz City of Science and Technology, Saudi Arabia

This study was undertaken to investigate the thermal behavior of nano-coatings of window glazing in a glazed test room for the regional conditions of Saudi-Arabia. Well controlled antimony doped tin oxide thin films on glass substrates were prepared using the aerosol-assisted chemical vapor deposition process to evaluate the films for solar control glazing applications. The optical and thermal properties of the films were measured and systematically investigated. The influence of antimony doping levels on absorption and reflection of solar radiation is examined with respect to the optical properties in the visible and near infrared spectra range. Glass U-factor, Solar Heat Gain Coefficient (SHGC), temperature distribution and net heat transfer through the glazed walls inside the room were calculated through numerical simulations. The experimental and numerical results obtained indicate that the nano-coating thickness and doping level concentration of ATO has pronounced effect on the thermal insulation of the window glass. It was noted that the overall transmittance of solar radiation in the visible, infrared and ultraviolent spectra regions decrease with increase of doping level of antimony tin oxides and increase of coating thickness. It was observed that the net heat transfer through the glazed walls of room decreased exponentially with increase of coating thickness or doping level concentration. Finally, from the analysis of results it was concluded that the antimony doped tin oxide thin films show outstanding optical and thermal properties and in comparison, to commercially available glazing, an improved solar blocking behavior is observed for nanostructured ATO thin films.

Speaker Biography

Ahmed M Almogbel has over fifteen years of teaching in research, management and training in different areas of mechanical engineering, including power, materials, design and manufacturing. He has 15 technical papers to his credit and supervised 7 graduation projects in various areas of heat transfer, fluid mechanics, air conditioning manufacturing and science of materials. He is specialized in air conditioning systems, human thermal comfort inside the building envelope and thermal insulations. He is currently conducting applied researches in solar air-conditioning system, desiccant-evaporative cooling technology, and energy performance optimization for hot and dry air conditioning systems. Ahmed is the principle investigator for the running strategic project in KACST about the solar adsorption air conditioning system.

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Influence of loose powder sintering parameters on the physical and the mechanical characteristics of bronze filters used at high pressure

Shaira M

National Institute of Applied Sciences of Lyon, France

Use of high-pressure bronze gas filters strictly requires certain physical and mechanical characteristics. Powder metallurgy technology is generally used as a method of manufacturing of filters; this method can easily ensure the high porosity for these materials; since sintering of the compact powders can lead to the creation of such porous structure, it can link between all particles and make them as a solid one. In the case that those filters maybe submit to extreme working conditions, they must be checked and tested according to specific test and characterization standards. Control of powder sintering parameters is therefore very important to warranty the good characteristics of those filters. In this context, a powder sintering method was chosen to elaborate such filters; loose powder sintering was used, and different parameters of sintering were applied. Each time, two objects were prepared in the sintering molds, they are the filter and a traction sample. Then, they were tested according the standards recommendations. The acceptable filters were only that respect all recommendations. Good results were obtained, and a very good protocol of sintering was identified.

Speaker Biography

Shaira M has completed his PhD in 2006 from INSA of Lyon, France. He is an associate professor at Al-Baath University, Syria, until 2017, and he is a visiting professor at INSA of Lyon. He has over 25 publications (journals, books at conferences), with an experience of more than of 17 years in teaching and research in several universities. He is a member of review committee of Journals of Engineering Science for the Universities of Al-Baath, Syria. He is also an editor in the academic journal of engineering sciences, USA.

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