2438th Conference

5th International Conference on

Theoretical, Materials and Condensed Matter Physics

November 26-28, 2018 | Los Angeles, USA

Plenary Talk

Day 1

Barbara A Jones, Res. Rev. J Mat. Sci. 2018, Volume 6
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Barbara A Jones

IBM Research – Almaden, USA

Emergent magnetism in the titanium nitride

Titanium nitride (TiN) is a well-known technological material, a heat insulator of extreme hardness, used in high-performance coatings on other metals, as well as a non-toxic material for medical applications. It is also extensively used in the microelectronics industry. In none of these applications is it magnetic. However, in our first principal's density functional calculations we show that when TiN is strained by increasing the separation between atomic layers, resulting monolayers of TiN become magnetic. We show how this magnetism is activated or emergent as the layer separation gradually increases: at a critical separation, the magnetism turns on, and remains magnetic in a stable configuration. We also show how this may be experimentally realized, with the addition of, for example, Argon into TiN, to create TiN monolayers either in the bulk or at the surface. In addition, our analysis leads to an understanding of the source of magnetism in TiN monolayers, even in the midst of bulk TiN, and only separated from the bulk by monolayers of Ar. We present 3D illustrations of those wave functions and orbitals responsible for the magnetism and the effects of other layers on this magnetism. We also show some related model systems which show unexpected magnetic behavior.

Biography

Barbara A Jones has been at IBM Almaden since 1989, working in a variety of areas from modeling magnetic recording devices to magnetic atoms on surfaces as studied by STM. She got her PhD from Cornell University in 1988, followed by a Postdoc at Harvard. She is on the Board of Physics and Astronomy of the National Academy of Sciences, an officer of the Physics Section of the AAAS, and an Honorary Member of the Aspen Center for Physics. She has been on the Editorial Boards of Physical Review X, Physical Review B, and Journal of Low-Temperature Physics.

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Day 1

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High-efficiency organic photovoltaics: Current and beyond

Sheng-Yung Chang and **Yang Yang**
University of California Los Angeles, USA

Organic photovoltaics (OPV) has become a promising alternative energy due to the light-weight property and environmental friendliness. In the past 20 years, its stabilized power conversion efficiency increases from less than 1% to higher than 10%, which is a remarkable accomplishment. The fundamental science inside the OPV device is thus an interesting and meaningful topic. To incorporate more innovative ideas to this growing field, the history of OPV development and the design strategies for improving the efficiency will be introduced in the first part of this topic. We are also going to present the works of the most updated world record-breaking OPV, which are designed by the UCLA team and certified by National Renewable Energy Laboratory. In the second part, we like to discuss the new and thriving trend for organic photovoltaics: high performance transparent organic PV (TOPV). Transparent photovoltaics, including building-integrated PV and agriculture-integrated PV, are recently receiving more attention due to their unique potential in future applications beyond just harvesting solar energy. TOPV, which is a branch of transparent PV, has several intrinsic superior physical and chemical properties for achieving transparency and further application. In order to stimulate more creative thinking in the transparency module and its application, our new works and discussion of advanced TOPV will be presented.

Biography

Sheng-Yung Chang is a fourth-year PhD candidate in the Department of Materials Science and Engineering, UCLA. His research interest focuses on organic electronics, including organic photovoltaics, light emitting diode, and sensor. He has been awarded the MOE Technologies Incubation Scholarship for 3 years and Enli-Tech Scholarship for 1 year for his excellent research performance. He has published more than 15 papers as first author or co-author in SCI journals as of November 2018.

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Chromatic and polychromatic radiation for crystal orientation

Danut Dragoi and **Alexandru Dragoi**
Non-affiliated Senior Scientist, USA

Modern Physics and Materials Science need a variety of innovative methods for characterization of materials. X-rays served as the best radiation for determining the orientation of single crystals, one important step in many advanced technologies in semiconductor industries and other. In the presentation, we will discuss the usage of both kinds of radiation, monochromatic and polychromatic in achieving the goal of determining high accuracy and precision for determining crystal orientation. The exact equation of orientation for both cases will be given along adequate parametrizations very useful in applications.

Biography

Danut Dragoi has completed his PhD at the age of 47 years from the University of Denver and postdoctoral studies from California Institute of Technology. He worked in Academia and Industry. He retired this year. He has published more than 70 papers in reputed journals and two books, one at Amazon and the other on Scholars' Press.

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Hari Datt Pandey, Res. Rev. J Mat. Sci. 2018, Volume 6
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Estimating vibrational lifetime and boundary conductance

Hari Datt Pandey
University of California Riverside, USA

Estimating vibrational signatures of a large molecular system is even tricky because of overlapping frequencies. Therefore, the vibrational probes are used to distinguish the vibrational signatures in the IR experiments. The underlying anharmonic interactions and prevailing resonances within the energy space dictate the vibrational lifetime, localization, participation, and energy flow pathway. These processes can be estimated from the quasiharmonic approximation accounting the intramolecular vibrational energy redistribution (IVR). The IVR process is irreversible and collisionless within the specified timescale of interest. We computed the IVR properties of liquid alkylbenzene systems by solving the vibrational Hamiltonian with the potential up to cubic or quartic anharmonic terms deriving the self-consistent system of nonlinear equation[1-3]. Only addressing the modes of interest and solving iteratively, the vibrational properties can be computed. Later we estimated the vibrational lifetime of the isotopically substituted nitrile probe, cyanophenylalanine[4-5]. The frequency of the nitrile of the four isotopomers decreases in the order $^{12}C^{14}N$, $^{12}C^{15}N$, $^{13}C^{14}N$, and $^{13}C^{15}N$, whereas the corresponding lifetime varies nonmonotonically with the change in frequency. The estimated lifetime first two C-N stretches are within 15% of the experimentally measured value 4.0, 2.4, 2.0, and 3.7 ps respectively and the other two are off by a factor of 2.[4-5] In the unsubstituted, $^{12}C^{14}N$, the coupled state are nonresonant at the level of cubic anharmonic interaction, whereas in other cases the energy flow is via the resonantly coupled pathway. The lifetime of $^{13}C^{15}N$ is slower contradicting the general convention that closer the resonance, faster the energy flow. We found that for some resonantly coupled modes to the CN are localized to the ring, while at other they are more delocalized. The resonantly coupled states are localized bright states and preferably is the reason behind the longer lifetime of the isotopically substituted case[4]. The IVR estimation method is also useful to determine the many-body localization-thermalization transition to estimate the boundary conductance. We have estimated the boundary conductance of various metal-alkane/perfluoroalkane-sapphier, metal-polyethylene glycol (PEG) oligomer junctions, and the results also agree with the experiments [6-11].

Biography

Hari Datt Pandey has completed his PhD in 2018 from University of Nevada Reno, USA and currently a Postdoc at University of California Riverside. He has published more than ten publications in his graduate study. His was involved in research of vibrational energy flow, and boundary conductance in the field of condensed matter physics. He was also involved in the dynamics of soft matters and currently participating in a conformational study of the protein, drug designing, and binding kinetics.

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Notes:

Jan Smotlakha, Res. Rev. J Mat. Sci. 2018, Volume 6
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Effect of the grain boundaries on the electronic and mechanical structure of graphene

Jan Smotlakha
Joint Institute for Nuclear Research, Russia

The grain boundaries in the graphene nanostructures usually consist of a combination of pentagonal and heptagonal defects. Being not very thick, they create regions of size tenths of nanometers. They arise during the production process and are intimately connected with the internal structure of the corresponding materials. The production process is mostly initiated by the chemical vapor deposition. Of course, the grain boundaries have a huge, usually undesirable influence on the electronic structure of the materials. Depending on the external conditions during the production, there can be qualitative differences in their properties. The resulting structures contain grains of different sizes, distributions and lattice orientations. Numerical calculations for a few samples were performed where the average sizes of the grains fluctuated from 13 to 25nm. They showed a considerable difference in the conductivities and charge carrier mobilities. The mobilities depend on the size of the grain boundaries linearly. Next, different configurations of the defects in the grain boundaries were considered and the corresponding polycrystalline structures showed significant differences in the investigated characteristics.

Biography

Jan Smotlacha has completed his PhD at the age of 33 years from Czech Technical University. Now he works as the senior research scientist in the Bogoliubov Laboratory of Theoretical Physics in the Joint Institute for Nuclear Research in Dubna. His investigation is concentrated on the graphene and other kinds of nanostructures and Weyl semimetals. Besides the electronic and magnetic properties, he models the influence of the structure perturbations connected with the topological defects and geometry. He has published about 20 papers in reputed journals or conference proceedings.

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U P Verma et al., Res. Rev. J Mat. Sci. 2018, Volume 6
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Electronic, mechanical and thermoelectric properties of Gd-filled ternary skutterudites

U P Verma, Shashank Nautiyal and **Priya Yadav**
Jiwaji University, India

Rare earth filled ternary skutterudite compounds have potential applications to produce clean energy, long-term stability and low cost as compared to other thermoelectric materials. For good efficiency, materials should possess high electrical conductivity, low thermal conductivity, and high Seebeck coefficient. In this communication, the electronic, mechanical and thermoelectric properties of Gd-filled skutterudites $GdFe_4P_{12}$, $GdRu_4P_{12}$ and $GdOs_4P_{12}$ have been reported. The study is based on full potential linearized augmented plane wave method in the framework of density functional theory. The exchange-correlation potential are treated using the generalized gradient approximation. The electronic behavior of this material is semi-metallic. Investigation of mechanical properties shows that reported materials are brittle and anisotropic. $GdOs_4P_{12}$ is stiffest among GdT_4P_{12} (T=Fe, Ru, Os). The Boltzmann transport theory with constant relaxation time has been used, as implemented in BoltzTraP code, to predict the thermoelectric properties of all the materials. The magnitude of Seebeck coefficient in spin down channel is more than that in spin up the channel. The maximum values of the figure of merit obtained in spin up channel are 0.44, 0.89 and 0.86 whereas in spin down channel the figure of merit are found to be 0.98, 0.90 and 0.96, respectively for $GdFe_4P_{12}$, $GdRu_4P_{12}$, and $GdOs_4P_{12}$. On the basis of the values of ZT, $GdRu_4P_{12}$ is efficient material in spin up configuration and $GdFe_4P_{12}$ in spin down configuration. Study of the electronic charge density shows that in the rare earth filled ternary skutterudite compounds have P-P covalent and Gd-B and Fe-B ionic bonding.

Biography

U P Verma has completed His PhD at the age of 25 from Meerut University, Meerut. He is the recipient of Alexander von Humboldt Fellowship at Justus Liebig University, Giessen and Goethe University Frankfurt. He has served as Regional Director of MP Bhoj Open University, Director Institute of Distance Education and as Head, School of Studies in Physics of Jiwaji University, Gwalior. He has published more than 100 research papers in journals of repute and supervised to 18 students for their PhD.

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Structural and magnetic properties of $Bi_{0.80}Ba_{0.20}Fe_{1-x}Ti_xO_3$ ceramics prepared by planetary ball milling technique

Feroz Alam Khan and **M S Rana**
Bangladesh University of Engineering and Technology, Bangladesh

The $Bi_{0.80}Ba_{0.20}Fe_{1-x}Ti_xO_3$ ($0 \leq x \leq 0.10$) ceramics samples are synthesized by solid state reaction and planetary ball milling technique. The structural, magnetic and electrical properties have been investigated over an wide range of temperature and magnetic field. It is observed that a structural phase transformation has occured for 20% Ba doped BFO. The rhombohedral crystal structure is transformed into a pseudo cubic structure causing a change in the unit cell volume and also that of the nanocrystalite. The FESEM images taken in different magnification shows that the grains are segregated into different clusters with a wide range of size distribution from 100-300 nm. The composition was later doped with Ti to observe the effect of Ti doping on the magnetic and electrical properties of the material.The dc magnetization shows that Ba doped Bismuth Ferrite samples is ferromagnetic with a significant magnetization. However with increasing Ti concentration the magnetization has decreased. The low temperature hysteresis shows diamagnetism for 10% Ti concentration which is regarded as a magnetic phase transition making this composition an interesting material for technological application. It is observed that the highest magnetization is achieved for 20% Ba doped BFO which indicate that there is a possible suppression of long cycloidal spin structure resulting in an enhanced magnetization. The introduction of Ba^{2+} ion at Bi^{3+} site is likely to induce oxygen vacancy which is one of the origins of leakage current. The change in orientation of FeO^6 due to the change of coordination of Fe is also assumed to be another origin of leakage current .We predict that the introduction of Ti^{4+} ion at the Fe site compensates for the oxygen vacancy and reduce the leakage current. In addition the introduction of Ti^{4+} is likely responsible for the increased resistivity of the material. The measured ac dielectric constant, dielectric loss, ac permeability at different temperatures show a strong frequency dependent behavior. The room temperature dielectric constant and dielectric loss factor have shown high values at low frequency and have decreased rapidly with increasing frequency.

Biography

Feroz Alam Khan has completed his PhD degree from the Bangladesh University of Engineering and Technology (BUET) and his Postdoctoral Research at the University of Delaware, USA, University of Uppsala, Sweden, and the University of Tsukuba, Japan. He is a Professor in Physics at the Bangladesh University of Engineering and Technology (BUET). He is a leader of a research group called Dhaka Materials Science Group under a scientific research collaboration with the International Science Programs (ISP), Uppsala University, Sweden. He has supervised more than 25 postgraduate degrees that include Masters, MPhil, and PhD degrees. He has to his credit more than 50 research publications. He is involved in promoting basic science research through the establishment of regional research collaborations with the south-east Asian Universities under the umbrella of International Science Programs.

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John Owen Roberts, Res. Rev. J Mat. Sci. 2018, Volume 6
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John Owen Roberts

Independent Researcher, UK

Implications of the link between the periodic table and the standard model

The mathematics of quantum physics from the standard model using groups U(1)xSU(2)xSU(3) and the Pauli Principle produces two sets of time independent quantum states n(n+1) and n(n-1) where n is the principal quantum number. Oscillations between these states result in a one to one mapping with the Roberts-Janet Nuclear Periodic Table by interpretation of n>0 for condensed matter and n<0 for plasma prior to fusion. The mechanism provides a framework for Periodic Tables for every supernova by excluding mass number. In the lower half of the table occupation by bosons leads to increased energy densities in which an ensemble of outcomes is discussed. A hypothesis of string theory is proposed at the nuclear end of the table merging into quantum loop gravity at the condensed matter top end of the table.

Biography

John Owen Roberts graduated in 1969 with a BSc (Hons) in Physics from The University of Liverpool. He has been an Open University Tutor for 30 years and a private tutor of Maths and Science. He is the author of "Those Infinities and the Periodic Table" (ISBN 978-0-9934667-3-1). He has had published an article "Proposed Link between the Periodic Table and the Standard Model", July 2017 in the Journal Materials Science and Engineering.

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Scientific Tracks & Abstracts

Day 2

Si-Han Chen, Res. Rev. J Mat. Sci. 2018, Volume 6
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Molecular dynamics investigation of surface potential and electro-kinetic phenomena at the amorphous silica/water interface

Si-Han Chen
The Ohio State University, USA

The static and electro-kinetic properties of amorphous silica-aqueous electrolyte interface are of long-standing scientific interest and current technological relevance. Different theoretical models of the electrical double layer (EDL) have been used to explain a wide range of experimental measurements, including zeta potential, second harmonic generation (SHG), sum frequency generation (SFG), electro osmotic flow (EOF), and streaming potential. Using extensive molecular dynamics simulations, we have studied this EDL as a function of salt concentration for a silica surface charge density of -0.82e/nm^2 (e=electron charge). The simulation results can be captured with a simple model by breaking the double layer region into three zones: an inner region in which the Na^+ counter-ion population is independent of [NaCl] and there are no Cl^- co-ions, an intermediate region which hosts a population of non- exchangeable Na^+ plus another group of Na^+ and Cl^- ions whose population is described by a Langmuir adsorption model, and an outer region where the ion distribution is well-described using Poisson-Boltzmann theory. To compare the applicability of our and other EDL models, e.g. the Gouy-Chapman, the constant-capacitance, and the triple-layer models, we analyze experimental data of SHG and streaming potential. We investigated the implications for interpretations of the results using different models, and scrutinize the correctness of the underlying physics.

Biography

Si-Han Chen has completed his PhD at the age of 32 years from the Ohio State University and he is now a postdoctoral researcher from the University of California, Riverside. He has published more than 7 peer-reviewed papers in experimental and theoretical chemistry. His current research field is binding kinetics of enzyme using machine learning-based methods.

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Thomas E Kodger, Res. Rev. J Mat. Sci. 2018, Volume 6
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Moldable soft polymers through topology

Thomas E Kodger
Wageningen University & Research, The Netherlands

Man-made rubbers, have excellent mechanical toughness but are inherently stiff due to topological constraints are known as entanglements, which prevent polymer chains from crossing and act as crosslinks. Thus, entanglements place a theoretical lower bound on how soft elastomers can be made without adding liquid fillers; soft materials with Young's moduli, E<0.2MPa are composed of multiple components and are not chemically pure substances. By introducing liquid fillers to polymeric materials, the stiffness may be decreased, however, this swollen material is mechanically brittle and leaks the filler material upon deformation inhibiting their use in many applications. Additionally, this swelling with solvent hinders their ability to be formed or molded into structures. In this talk, I will discuss the synthesis of soft, moldable elastomers. This material is synthesized using controlled living polymerization techniques to fabricate a triblock copolymer with a middle block of silicone polymers in a 'bottlebrush' architecture which eliminates entanglements making the material soft without the necessity for the solvent. The triblock polymer includes functional end blocks composed of a thermoplastic, polystyrene, which undergoes a glass transition upon cooling, allow this material to thermoset reversibly, that is 3D printed. I will present the synthesis and mechanical characterization of this material and high-resolution 3D printing of finely detailed soft structures.

Biography

Thomas E Kodger completed his PhD from Harvard University in 2015 under Professor David Weitz and Postdoctoral studies from the University of Amsterdam with Professor Peter Schall. He is currently an Assistant Professor in the Physical Chemistry and Soft Matter Laboratory at Wageningen University & Research in The Netherlands having joined in 2017.

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Electronic properties of Mn-decorated silicene and other 2D materials

Barbara A Jones
IBM Research – Almaden, USA

We first discuss silicene on hexagonal boron nitride, using first-principles calculations. Since hexagonal boron nitride is semiconducting, the interaction with silicene is weaker than for metallic substrates. Therefore, it is possible to open a 50meV band gap in the silicene. We further address the effect of Mn decoration by determining the onsite Hubbard interaction parameter, which turns out to differ significantly for decoration at the top and hollow sites. The induced magnetism in the system is analyzed in detail, and we compare and contrast with the behavior of other pairings of magnetic adatoms and 2D surfaces.

Biography

Barbara A Jones has been at IBM Almaden since 1989, working in a variety of areas from modeling magnetic recording devices to magnetic atoms on surfaces as studied by STM. She got her PhD from Cornell University in 1988, followed by a postdoc at Harvard. She is on the Board of Physics and Astronomy of the National Academy of Sciences, an officer of the Physics Section of the AAAS, and an Honorary Member of the Aspen Center for Physics. She has been on the Editorial Boards of Physical Review X, Physical Review B, and Journal of Low-Temperature Physics.

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Density matrix in the description of the collision of an atomic particle with a solid film

Gennadiy Filippov
Chuvash State Pedagogical University, Russia

Calculation and further analysis of density matrix (DM) for a projectile which collides with a solid film reveal some new representations which hard to be anticipated without the calculation. Namely:

1. The coherence properties in the projectile's wave field are describing through the special function of coherence. $f(\vec{x}_1,\vec{x}_2,t)=\frac{2\Gamma(\vec{x}_1,\vec{x}_2,t)}{\Gamma(\vec{x}_1,\vec{x}_1,t)+\Gamma(\vec{x}_2,\vec{x}_2,t)}$, where $\Gamma(\vec{x}_1,\vec{x}_2,t)$ - density matrix of the projectile depending on two spatial points $\vec{x}_1,\vec{x}_2$ and the time *t*.

2. The collision with the solid leads to a significant decrease in the total coherence length of the projectile's wave field. The coherence length can become much smaller than the initial size of a wave packet of a particle passing through the film.

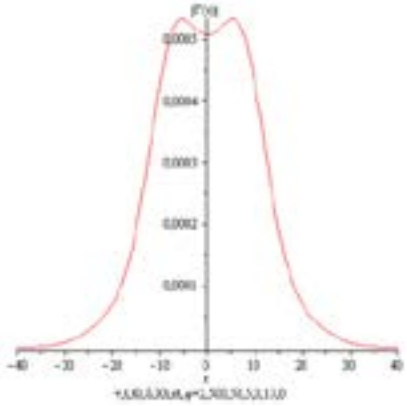
3. During the collision with solid, the number of different spatial areas where the mutual coherence in the projectile's wave field is supported can be multiplied.

4. Every part of projectile's wave field can be individualized as the separate particle having own property in its inner quantum state. The procedure which has a responsibility for such a transformation can be characterized as a spontaneous breaking of symmetry.

5. The process described in point 3 can be considered as a special form of breaking in quantum mechanics.

6. Knowing the wave packet evolution during the passage through the solid film allows one to explain experimental results on the pore formation during the passage of high charged atomic ions through the thin carbon nano-membranes.

7. The parts of the wave field considered above can be stabilized in its quantum state after been captured in its own polarization well.



Biography

Gennadiy Filippov has his expertise in particle-solid interaction physics. He has completed his PhD at the age of 54 years from Tomsk State University (Russia). He is head of the Laboratory of Biophysics and Bio-nanotechnology in the Chuvash State Agricultural Academy and professor in the Chuvash State Pedagogical University in Cheboksary, Russian Federation.

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Seismic imaging of soils for slope stability in Ngoketunjia division, Northwest region, Cameroon

Paul Leifeh Njuabeh
The University of Bamenda, Cameroon

This study has been conducted around the Ngoketunjia slope in Ngoketunjia Division, Northwest region, Cameroon, West Africa, on the subject, seismic imaging of soils for slope stability in Ngoketunjia division. Subsequently, the probability of failure of the real slide in Ngoketunjia. The most valuable infrastructural assets of this division are aligned along the feet of these slope coupled with the habitual human activities and settlement, whereas findings of the stability of these slopes have not yet been ascertained. Following these highlights, we are likely to say that, both materials properties and human lives may be exposed to the risk of instability of the slopes. In this paper, we describe how state-of-the-art 3-D seismic data can be acquired, analysis, interpreted, integrated with other data and then used to improve the geographical design of the slope and ascertain its stability. The primary imaging targets were heterogeneous siltstone and fine-grained sandstone successions approximately 100ft (30m) thick and comprised of complex assemblages of thin lobe-like deposits having individual thicknesses of 3 to 6ft (1 to 2m). Secondary data was generated from a write-up that was examined in 2003 at the depth of approximately 6600ft (2000m) by The Upper Noun Valley Development Authority. A geographical survey was conducted on the slope, followed by three soil test (identification, characteristics, and porosity) that were conducted on soils sample collected in strata from the slope. The effect of various parameters including slope inclination angle, the angle of internal friction of soil, horizontal seismic loading, the cohesion of the silos and surcharge loading has been examined. After analyzing our results, we found out that the stability of a sloping soil is largely affected by the horizontal seismic forces. We show by the careful consideration that, given the prevailing climatic changes that keep increasing the water table content of the slope year by year, thereby increasing the porosity of the soils may lead to the failure of the slope. Secondly, the habitual human activities like excavations and construction, which keeps increasing the load sustained by the slope have led to a drastic increase in the driving forces along the different sections of the slope and consequently the factor of safety. Mitigation measures like bio-restoration, drainage systems, retaining walls, rock bolting were advised to the municipality of Ndop Central Sub Division. The cost of carrying out the study, lack of potable or mobile equipment to use during the study and the unavailability of related publications were some of the limitations to the study and we are proposing that further research works should take into consideration these limitations in other to address major global concerns in this area of study.

Biography

Paul Leifeh Njuabeh, is a holder of an Executive MBA in management and a prospective MSc in Condensed matter physics, his age of 28 years from Bamenda University. He is serving at the Ministry of public contracts Cameroon as the chief of bureau for Infrastructural contracts in Ngoketunjia Division, Cameroon. Before joining the Ministry of public contracts, he has earlier serve at the Ministry of Education Cameroon as an instructor and a statistician.

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Cooper pairs in superconductivity in a generalized BEC theory

I Chávez, LA García, M Grether and **M de Llano**
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The generalized Bose-Einstein condensation (GBEC) theory subsumes as special cases both BCS and BEC, among other theories. It hinges on three separate new ingredients: i) treating Cooper pairs (CPs) as *actual* bosons as distinct from BCS pairs which strictly speaking are not bosons; ii) inclusion of two-hole Cooper pairs (2hCPs) on an equal footing with the usual two-electron ones (2eCPs); and iii) incorporating in the resulting ideal *ternary* boson-fermion (BF) gas specific vertex interactions that drive formation/dis-integration processes of both kinds of CPs. Here we extend the BCS-Bose crossover theory by *explicitly* including 2hCPs. This leads to a phase diagram with two pure phases, one with 2eCPs and the other with 2hCPs, plus a mixed phase with arbitrary proportions of both. The special-case phase with a 50-50 mixture of both 2e/2hCPs gives the usual *unextended* BCS-Bose crossover theory. Furthermore, if T_c and T_F are respectively the critical and the Fermi temperatures, it predicts T_c/T_F values for the elemental superconductors Al, In, Sn, Pb, Hg, and Nb comparing quite well with experiment and notably much better than BCS predictions. Also shown is a phase diagram of the dimensionless energy gap at zero-temperature $\Delta(0)/E_F$ *vs* n/n_f, where $E_F=k_BT_F$ is the Fermi energy. We do this for the 50-50 case as well as for the pure 2eCPs and 2hCPs cases separately. It is thus unequivocally shown that if one ignores 2hCPs the energy gap lies substantially below the 50-50 case which already roughly reproduces the data.

Biography

I Chávez MS and BS have completed his Doctoral degree in the Material Sciences and Engineering Research Graduate Program at the National Autonomous University of Mexico (UNAM, in Spanish) with the thesis titled "*A new dimensionless coupling constant in superconductivity*." He is also a Laboratory Assistant at the School of Sciences at UNAM.

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Toward rational design of new photocatalytic materials for solar fuel generation using density functional theory

Moussab Harb and **Luigi Cavallo**
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Solar hydrogen production through the challenging photocatalytic water splitting using powder semiconductor materials still remains a promising technology due to the low cost required. Designing new potential absorber semiconducting materials used in visible-light-driven photocatalytic water splitting cells requires the appropriate determination of different components that will be assembled in the final device. In addition to the required good chemical stability in aqueous solution, high crystallinity and adequate band gap energy of the prepared material (greater than 1.23eV and near 2.0eV) to absorb a wide range of photons in the visible region, which counts for 43% of the solar spectrum, other specific intrinsic parameters directly involved in the processes must be properly tuned. They include the solar light absorption intensity, exciton binding energy, the possibility of charge carrier diffusion throughout the crystal structure to the surface and their interaction with the solution. Experimentally, previous works on semiconductors widely used in photovoltaic devices revealed that high dielectric constant is needed to obtain a good ability for exciton dissociation into free holes and electrons at room temperature. A delocalization orbital character of photogenerated charge carriers is also required to give low effective masses and help for their good transport to the surface by minimizing the electron-hole pairs recombination. Moreover, suitable valence band (VB) and conduction band (CB) edge positions with respect to water redox potentials are also needed to give the driving force to the photogenerated holes and electrons to oxidize water and to reduce H^+. To design and characterize new materials for solar energy conversion applications, the density functional theory (DFT) has emerged as a valuable computational tool to quantify these key intrinsic parameters because of the difficulties to their direct experimental measurement. Achieving accurate DFT computations is thus particularly relevant, and this is known to be in strong correlation with the type of the exchange-correlation functional used to describe the various electron-electron interactions. In previous theoretical studies on largely utilized semi-conducting materials in photocatalytic water splitting and photovoltaics, we have shown that the intrinsic parameters mentioned above can be predicted with good accuracy using DFT along with the screened Coulomb hybrid Heyd–Scuseria–Ernzerhof (HSE06) functional. Following this robust computational protocol, we have shown suitable band edge positions for visible-light-driven overall water splitting of $(Ta_{3-x}N_{5-5x})O5_x$ ($x \geq 0.16$) compounds. Besides, we have predicted interesting dielectric, charge carrier transport and redox features of $(Ta_{1-x}Nb_x)ON$ solid solution materials ($0.25 \leq x \leq 0.5$) for water splitting while they revealed almost UV light absorption features due to their large predicted direct bandgaps in the 2.8-3.0eV range. Recently, we have predicted $Ta_{0.75}V_{0.25}ON$ as a promising photocatalyst for splitting of water driven by solar light, with an adequate band gap of 2.0eV, high absorption efficiency, a static dielectric constant greater than 10, smaller hole and electron effective masses than $0.5 m_0$ along the [001] and [010] crystallographic directions respectively, binding energy of the exciton lower than 25meV, and suitable energy levels of band edges for water splitting limits. The obtained solar energy absorption and redox features of $Ta_{0.75}V_{0.25}ON$ were clearly better than those acquired for Ta_3N_5, which is the most common semiconductor photocatalyst used in visible-light-driven water splitting. In my talk, I will first show how DFT can greatly help the experimentalists for a rational design of new photocatalytic materials for solar energy conversion by giving relevant information on key and recent examples. Secondly, I will present a deep DFT-based computational study successfully achieved recently in combination with experiment aiming to understand the nature of the trap states that are significantly decreased upon hydrogen treatment and explain the electronic origin of the charge carrier lifetime enhancement in bismuth vanadate ($BiVO_4$) through mild hydrogen treatment. Overall, these findings provide further insights into the interplay between defect modulation and carrier transport in metal oxides, which benefit the development of low-cost and highly-efficient solar energy conversion devices.

Biography

Moussab Harb has completed his PhD in 2008 at the age of 25 years from Light-Matter Institute (ILM) at Claude Bernard University (UCBL-France). Until 2014, he has completed several Postdoctoral research studies from Multidisciplinary Research Institute on Environment and Materials (IPREM-France), French Petroleum Institute (IFPEN-France) and KAUST Catalysis Center (KCC-KSA). He is currently a Research Scientist in Computational Physical Chemistry for solar Energy Conversion at KAUST University working on the Design of new potential and efficient 3D and 2D materials for visible-light-driven photocatalytic water-splitting and photovoltaic devices using accurate first-principles quantum calculations. He has published more than 50 papers in peer-reviewed journals and has been serving as a member of ACS, APS, AIP and MRS societies and reviewer of many relevant scientific journals.

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Fabrication and characterization of copper doped cadmium sulphide thin film solar cell

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The fabrications of electronic components, especially solid-state devices and microelectronic integrated circuits, have undoubtedly found the widest and most demanding applications for thin-film depositions. With a view to fabricating a solar cell, a prepared precursor of Copper Cadmium dithiocarbamate was used for the deposition of CuCdS thin films at 420°C on ITO coated glass substrate by MOCVD technique as the absorber layer. Aluminium doped Zinc Oxide (AZO) was also deposited by spray pyrolysis at 350°C as the window layer on the deposited absorber layer. Silver paste was drop-dried on the deposited window layer as the ohmic contact. The result of the deposited layered thin films and the solar cell were analyzed using Rutherford Backscattering Spectroscopy and Energy Dispersive X-ray (EDX), UV Visible spectrophotometer, Keithley four-point probe instrument, and I-V analysis. The RBS analysis of the deposited CuCdS film revealed the percentage composition of Cu=4.20%, Cd=10.77%, S=33.74%, and O=51.27%. Film thicknesses of 133nm and 889nm were recorded for AZO and CuCdS thin film respectively as obtained from the RBS analysis. The composition of AZO as observed by EDX is Al=1.13%, Zn=66.40%, and O=21.61%. The UV-visible analysis of AZO film revealed that the film had an optical transmittance of 60% in the visible portion of the spectrum with a direct bandgap of 3.25eV, while bandgap of CuCdS is 2.41eV. The absorbance of the CuCdS film was observed to be low in the VIS/NIR regions and high in UV region. The sheet resistance and resistivity of AZO film are 9.58×10^{6} Ω/square and 1.27×10^{-2} Ωcm respectively, while 1.17×10^{9} Ω/square and 10.40Ωcm were obtained as the sheet resistance and resistivity of CuCdS film respectively. The I-V analysis of the fabricated solar cell showed that, under dark condition, it behaves like a diode or semiconductor current rectifier. The fill factor as extracted from the device and its corresponding conversion efficiency are 0.6911 and 4.38% respectively.

Biography

Sabur Abiodun Ayinde is a PhD student at Obafemi Awolowo University where he had his masters in Engineering Physics in 2015. He is a 33 years academic staff of The Federal Polytechnic, Ede, Nigeria. He has worked in a manufacturing industry after the graduation of his first degree and has spent the past 7 years of his life as a polytechnic teacher. He has attended a series of conferences and has published more than 8 papers in reputed journals. In his quest to know how things work, he likes to solve challenging problems in materials and solid state electronics. He is happily married with a kid and has always had the desire to render community services to the people.

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Determination of mechanical, structural and thermodynamic properties of the half-heusler compound (Zirconium Lead Palladium) in solid state physics

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Half-Heusler compounds are promising semi-conductors which are environmentally friendly and of low-cost thermoelectric materials. They have a high figure of merit. Half-Heusler (HH) alloys are among the most promising novel thermoelectric (TE) materials intended for mid-to-high temperature power generation applications. They are members of the vast family of Heusler alloys with the general composition X_2YZ, consisting of three interpenetrating face-centered cubics (fcc) sub-lattices (Wang et al., 2016). Zirconium Lead Palladium (ZrPdPb) is one of the examples of the Half-Heusler alloy that crystalizes in the face-centered cubic structure with the space group F4-3m (Koller *et al.,* 2009).In this work, the structural, mechanical and thermodynamic properties of ZrPdPb were investigated by the first-principle calculations using Quantum Espresso that implements the Density Functional Theory (DFT). The results indicate that all Half-Heusler compounds are narrow-gap semiconductors. The results of Young's modulus, elastic constants C_{11}, C_{12} and C_{44}, Shear modulus, and Lattice constants, Bulk modulus and pressure derivative which constitute the mechanical and structural properties respectively of ZrPdPb are in good agreement with the results in the literature. The thermodynamic properties of ZrPdPb such as Heat capacity, internal energy, entropy, free energy, Debye temperature etc. were calculated using Quantum Espresso. It is seen that at room temperature i.e. 300k, the internal energy is 23.15kJ/(molk), and the heat capacity is 72.27kJ/(molk). The Debye temperature is found to be 365.3K. From 500K and above, the heat capacity approaches an asymptotic value of 37J/mol/K and obeys Dulong-Petit law which states that at high-temperature Specific heat capacity of a substance remains constant. Also, at sufficiently low temperature, the specific heat capacity is proportional to T^3. The heat capacity of ZrPdPb shows that the Half-Heusler alloy has little electrical and thermal conductivity as greater heat energy is required to break the intermolecular forces. The mechanical properties ZrPdPb show that the material is not stable under heavy vibration. Suggestions were made to improve the mechanical and thermodynamic properties. Other properties like the magnetic and optical properties of ZrPdPb should be studied. The electrical, mechanical and structural properties of ZrPdPb should be studied by alloying. The electronic, mechanical, structural, magnetic properties of ZrPdPb should also be studied under pressure.

Biography

Ogundola Sunday hails from Irele LGA, Ondo State of Nigeria. He bags BSc Ed in physics from Obafemi Awolowo University, Ile-Ife, Nigeria. He has MSc in Theoretical Physics from University of Benin, Nigeria. He has written some reputed the University-based journals in Nigeria. He is currently a Physics Lecturer at Federal College of Education, Eha-Amufu, Enugu state, Nigeria. He is eagerly opting for his PhD in University of Benin, Nigeria. He is happily married with three children.

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High-temperature solar cells

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The conversion of light to electricity can be done indirectly by first converting light to high-temperature heat and then heat to electricity or directly using solar cells. These processes are today carried out on a large scale in physically separate solar plants. The indirect process is limited by the thermodynamically dictated Carnot efficiency while the direct conversion efficiency has an upper bound the Shockley-Queisser limit. Is there a way to overcome these efficiency limitations without violating physical laws? Clearly, a way dramatically to lower solar electricity costs would be to combine both processes in a single solar power plant facility without substantially increasing its capital cost. Such a hybrid procedure would effectively double the conversion efficiency but it would require the use of solar cells that operate at 400 Centigrade or above. Such cells do not exist today and therefore this attractive approach cannot be implemented. This presentation focuses on recent breakthrough developments in condensed matter physics and chemistry that are anticipated to lead to the creation of a new generation of high-temperature solar cells. Spectacular advances have occurred in the synthesis and nanophotonics of wide band-gap (WBG) semiconductors as well as in understanding the unique quantum electrodynamic properties of graphene for which the 2010 Nobel Prize in Physics was awarded. The p/n heterojunctions between these two materials are predicted to allow very effective separation of electron/hole pairs formed in graphene by the absorption of the total solar spectrum waveguided along the length of the WBG nanowires. These materials were selected because their electronic structures are influenced only minimally by increasing temperature and because these materials are not resource limited as well as being environmentally benign.

Biography

Dieter M Gruen received his PhD at the University of Chicago in Chemical Physics. He is an Argonne Distinguished Fellow, Emeritus and President of Dimerond Technologies LLC. He is an internationally recognized scientist and innovator with more than 400 publications.

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Using the floquet-magnus and the Fer expansion approaches to control the spin dynamics in solid-state nuclear magnetic resonance and beyond

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The topic of the talk opens a way to an infinite number of suggestions. However, it is very important to remember that the spin dynamics have recently found new major areas of applications such as topological materials. Researchers, dealing with those new applications, are not usually acquainted with the achievements of the magnetic resonance theory, where those methods were developed more than thirty years ago. They repeat the same mistakes that were made when the methods of spin dynamics and thermodynamics were developed in the past. This talk focused on the spin dynamics in solid-state nuclear magnetic resonance (NMR) and beyond. This presentation is very useful not only for the NMR, physical, and chemical physics communities but for the new communities in several younger fields. It will be very useful for scientists working in different directions. In this talk, I will present the use of the Floquet-Magnus expansion and the Fer expansion approaches for the calculation of effective Hamiltonians and propagators in solid-state NMR. These approaches are very important and contribute theoretically and numerically in the general field of spin dynamics and chemical physics.

Biography

Eugene Stephane Mananga is the Deputy Executive Director of The CUNY ACADEMY FOR HUMANITIES AND SCIENCES, and a member in the Board of Directors-at-Large of The ACADEMY. He is a Faculty Member in the Physics & Chemistry Doctorate Programs at the Graduate Center of the City University of New York. He is an Assistant Professor of Physics and Nuclear Medicine at BCC of CUNY, and an Adjunct Professor of Applied Physics at New York University. He completed his Ph. D in Physics from the Graduate Center of the City University of New York, and holds 6 additional graduate degrees and training from various institutions including Harvard University, Massachusetts General Hospital, and City College of New York.

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