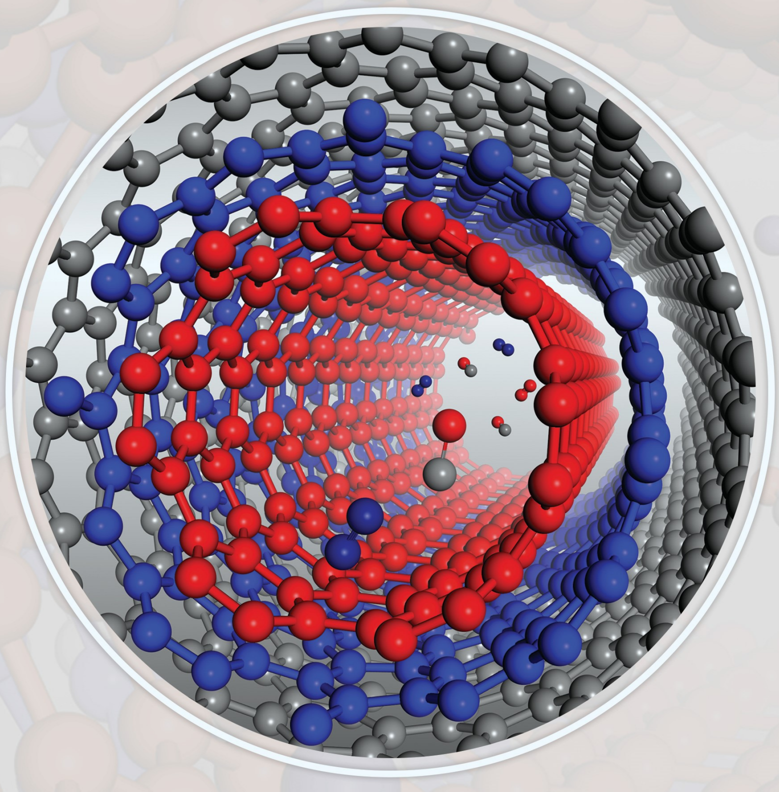
SRM
UNIVERSITY AP
Andhra Pradesh

INTERNATIONAL CONFERENCE ON MATERIALS GENOME
(ACCMS-ICMG-2020)
& FRACMEET-2020

SRM University - AP, Andhra Pradesh
5-7th February, 2020



In association with:
Asian Consortium on Computational Materials Science
Jawaharlal Nehru Centre for Advanced Scientific Research
Institute of Mathematical Sciences

Prof. D. Narayana Rao
Pro Vice Chancellor, SRM University-AP

MESSAGE

I am very glad that SRM University -AP in association with Asian Consortium on Computational Materials Science (ACCMS), Jawaharlal Nehru Centre for Advanced Scientific Research, Bengaluru and the Institute of Mathematical Sciences, Chennai are organizing a premier international event, ACCMS - International Conference on Materials Genome (**ACCMS-ICMG 2020**) at SRM University- AP from 5th to 7th February 2020. The importance of enormous leap in computational approaches followed by experiments over the past three decades will be discussed and the main focus is on the Quantum mechanics based calculations followed by Machine Learning technique (QM/ML) to predict new materials for various applications.

A special parallel conference, **FRACTMEET 2020** is organized to discuss the most recent standing of mechanics of porous media, granular systems, glassy and amorphous materials, bio-materials etc from the point of view of statistical physics.

Let me take this opportunity to thank the conveners, and the young brains for hosting the international conferences at SRM University -AP, which brings experts, students and researchers of computational methods together. I extend a warm welcome to all the participants.

I am extremely happy that two international peer reviewed journals, "The Journal of Electronic Materials" and "Catalysis Today", have accepted to publish selected papers in their respective Special issues of this conference.

All the sessions have been carefully planned to discuss about the current developments and key challenges in the research area of Machine learning for materials, electronic structure of materials using First-Principles calculations and fracture in materials.

I strongly believe that this joint venture would greatly benefit both the young research scholars and experienced faculty members in the field and I hope that this program would promote fruitful collaborations and further stimulate research activities in the field of computational materials genome.

(D. Narayana Rao)

Our History and Future

Yoshiyuki Kawazoe

New Industry Creation Hatchery Center (NICHe), Tohoku University, Aobaku, Sendai 980-8579, Japan, School of Physics, Institute of Science and Center of Excellence in Advanced Functional Materials, Suranaree University of Technology, Nakhon Ratchasima, Thailand 30000, and Department of Physics and Nanotechnology, SRM Institute of Science and Technology, Kattankulathur, Tamil Nadu-603203, India.

When we started ACCMS in Sendai, Japan in 2000, there were only 17 researchers gathered from 7 countries, but all of them were very active and we immediately recognized that it was an important meeting and started to organize a regular series of meetings every two years. At that time, there were no well-defined concept of computational materials science (CMS), and the subject was called theoretical solid-state physics or quantum chemistry. Therefore, it was a challenge for us to organize such a new group of researchers in Asian region. The first conference was successfully held in Bangalore in 2001 with 85 participants. We have discussed and decided that we should keep our originality and priority in CMS in Asian region by developing our own software and share them in ACCMS members. One of the software we have chosen is TOMBO (TOhoku Mixed Basis Orbitals *ab initio* simulation program package), which has been developed mainly by Prof. Ohno, based on a completely original idea of mixed-basis (system wave function is composed by plane waves and atomic orbitals). TOMBO has a number of advanced features what other existing *ab initio* software cannot treat, such as absolute energy estimation, GW+gamma approximation, chemical reaction tracing, and more. We have already organized a number of TOMBO tutorials to introduce these ideas and try to expand the users and developers in ACCMS community. Another important thing is that we should be able to predict new useful materials with confidence (not fit to the experimental observations). By this concept we can establish a fundamentally important position in materials science as “Theory First”, which is standard in elementary particle physics, which was my subject when I was a student.

In these 20 years of the CMS history, computer power has become improved tremendously (~10,000times) and realistic materials can be treated theoretically. However, unfortunately *ab initio* simulation has become more and more phenomenological and away from real first principles. We should be very careful, since only explaining the experimental observations (“Experiment First”), we are not necessary person in fundamental research (although welcome by experimentalists?).

In the 20 years of the history of ACCMS, 32 conferences have been held in 12 countries/regions, but there has been no real Centre and I have taken care of necessary things to maintain the consortium as a Virtual Organization (VO). Since CMS is very popular now, especially with the concept of Materials Informatics (MI), now is the time to establish our Real International Centre for the CMS researchers in Asian region, especially for young researchers to enjoy better environment such as in the International Centre for Theoretical Physics in Trieste. We, members of ACCMS, have discussed for quite a long time, and finally decided to settle it in SRMIST in Chennai. New era of ACCMS starts from 2020. Please keep on staying in ACCMS.

Fracmeet-2020: From the organizer’s desk

It is our great pleasure to organize Fracmeet 2020 at the SRM University - AP, in association with the Asian Consortium on Computational Materials Science (ACCMS). Fracmeet has been organized every year since 2011. The idea behind Fracmeet is to have a small meeting, with typically 30-35 participants, to provide a platform for intense discussion on the recent developments and future directions of various important aspects of mechanical behavior of complex and advanced materials. Chemists, physicists, material scientists, engineers and researchers from Industries have taken part in Fracmeet as participants and speakers. So far, Fracmeet has always been held at The Institute of Mathematical Sciences, Chennai, with the support from the Institute. This year, we wanted to organize it elsewhere and given the nature and the topics of the meeting, what can be more befitting than to organize Fracmeet as a part of ACCMS. We thank the organizers of ACCMS for providing us with the opportunity and the Physics department, SRM University - AP and The Institute of Mathematical Sciences, Chennai, for infrastructural and financial support. The topic of this year's Fracmeet is "Micro-mechanics of failure in disordered materials" and like past years we hope to have a fruitful and enjoyable meeting.

Soumyajyoti Biswas
Pinaki Chaudhuri
Purusattam Ray
(Conveners, Fracmeet-2020)

Program Schedule
ACCMS: International Conference on Materials Genome (ICMG-2020) & Fracmeet-2020

Venues for talks:

Plenary sessions: Hall-3, 4th floor, academic block
Blue sessions: Hall-4, 4th floor, academic block
Red sessions: Hall-3, 4th floor, academic block
Green sessions: Hall-1, 3rd floor, academic block (Fracmeet-2020)

5th February

8:30-9:30 Registration (4th floor, academic block, SRM University- AP)
9:30-10:00 Inaugural session

Chair: U. Schwingeschlögl ***(session - I)***	**P. Jena (10:00-10:30)** **Y. Kawazoe (10:35-11:05)**	
	Tea 11:05-11:30	
Chair: S. Narasimhan ***(session: II-A)*** G. P. Das (11:30-12:00) K. R. Lee (12:05-12:35) Lei Shen (12:40-13:10)	**Chair: E. Kwon** ***(session: II-B)*** U. Schwingeschögl (11:30-12:00) Amrita Bhattacharya (12:05-12:35) S. K. Ghosh (12:40-13:10)	Opening remarks (11:20-11:30) **Chair: B. K. Chakrabarti** ***(session: II-C)*** T. Hatano (11:30-12:15) A. Banerjee (12:20-13:05)
	Lunch 13:10-14:00	
Chair: K. R. Lee ***(session: III-A)*** Saurabh Ghosh (14:00-14:30) H. Mizuseki (14:35-15:05) A. K. Singh (15:10-15:40)	**Chair: G. P. Das** ***(session: III-B)*** S. Bhattacharya (14:00-14:30) P. Ghosh (14:35-15:05) P. Sen (15:10-15:40)	**Chair: P. Chaudhuri** ***(session: III-C)*** L. Goehring (14:00-14:45) A. Das (14:50-15:35)
	Tea 15:40 – 16:00	
Chair: P. Jena ***(session: IV-A)*** N. Duc (16:00-16:30) D. Prasad (16:35-17:05)	**Chair: S. Khanna** ***(session: IV-B)*** E. Kwon (16:00-16:30) M. V. M Jyothirmai (16:35-17:05) P. Banerjee (17:10-17:30)	**Chair: T. Hatano** ***(session: IV-C)*** R. Rajesh (16:00-16:45) C. Roy (16:50-17:15)

6th February

Chair: Y. Kawazoe ***(session-VI)***	**F. Kun (9:30-10:00)** **S. Khanna (10:05-10:35)**	
Tea 10:35-10:50		
Chair: R. Thapa ***(session: VII-A)*** S: Narasimhan (10:50-11:20) H. Yasumatsu (11:25-11:55) N. Zhanpiesov (12:00-12:30) M. Haider (12:35-13:05)	**Chair: N. Zhanpeisov** ***(session: VII-B)*** K. Hermansson (10:50-11:20) B. Nanda (11:25-11:55) S. K. De (12:00-12:30) H. Das (12:35-13:05)	**Chair: P. Ray** ***(session: VII-C)*** S. Tarafdar (11:00-11:45) A. Nakahara (11:50-12:35) S. Roy (12:40-13:05)
Lunch 13:05-14:10		
Chair: R. Maezono ***(session: VIII-A)*** K. Hongo (14:10-14:40) M. Dixit (14:45-15:05) A. Manjanath (15:10-15:30) T. Yang (15:35-15:45)	**Chair: D. Nguyen** ***(session: VIII-B)*** M. Ravva (14:10-14:40) V. Lee (14:45-15:15) V. Subramanian (15:15-15:45) K. Ulman (15:45-16:05)	**Chair: S. Tarafdar** ***(session: VIII-C)*** P. Tandaiya (14:10-14:55) S. Pradhan (15:00-15:25) (Skype) B. K. Chakrabarti (15:30-16:15)
Poster and Tea 16:00-18:00		
Banquet 19:30 -		

7th February

Chair: J. Siriporn ***(session: IX)***	**R. Thapa (9:30-10:00)** **R. Maezano (10:05-10:35)**	
Tea 10:35-10:50		
Chair: K. Hongo ***(session: X-A)*** T. Basak (10:50-11:20) M. Aziz (11:25-11:55) K. Joshi (12:00-12:10) A. Kumar (12:15-12:25)	**Chair: V. Lee** ***(session: X-B)*** K. Ramanujam (10:50-11:20) J. Siriporn (11:25-11:55) S. Kalluri (12:00-12:10) V. Arivindan (12:15-12:25)	**Chair: L. Goehring** ***(session: X-C)*** V. Madhurima (11:00-11:45) S. Karmakar (11:50-12:35) K. Vishwanathan (12:40-13:25) Closing remarks (13:25-13:30)
Closing remarks (12:45-13:15)		
Lunch 13:15-14:30		
Tour (14:30-18:00)		

Program Schedule
ACCMS: International Conference on Materials Genome (ICMG-2020)

Organized by ***SRM University – AP***
In association with
Asian Consortium for Computational Materials Science
Jawaharlal Nehru Centre for Advanced Scientific Research
Institute of Mathematical Sciences
5- 7 February 2020

5th February, Wednesday 2020

Venue: Hall 3 and Hall 4, 4th Floor, Hall 1, 3rd Floor Admin Block

8.30 a.m. to - 9.30 a.m.: Registration, 4th Floor, Academic Block, SRM University
9.30 a.m. - 10.00 a.m.: Inaugural Session

Morning Session: 10.00 a.m. – 1.00 p.m.
Session I – Morning Lecture – Single Session
Session Chair: Prof. Udo Schwingeschlögl, KAUST, Saudi Arabia

10.00 a.m. – 10. 30 a.m.	Hall 3	Invited Lecture 1	Prof. Puru Jena, VCU, USA	Title: In Search of Metastable Forms of Carbon
10:35a.m – 11:05 a.m	Hall 3	Invited Lecture 2	Prof. Yoshiyuki Kawazoe, Tohoku University Japan	Title: Theoretical Materials Research in Past and Future
11.05 a.m. – 11.30 a.m.	Tea/Coffee Break 25 mints			

Session II A – Parallel: Materials Prediction, Database and Framework
Session Chair: Prof. Shobhana Narasimhan, JNCASR, India

11:30 a.m. – 12:00	Hall 3	Invited Lecture 3	Prof. G. P. Das, IIT KGP, India	Title: Computational design of low dimensional materials for energy applications
12:05p.m. – 12.35 p.m.	Hall 3	Invited Lecture 4	Prof. K. R. Lee, KIST, South Korea	Title: SimPL: A Framework for Web-based Materials Design Platform
12:40 a.m. – 01:10 p.m.	Hall 3	Invited Lecture 5	Prof. Lei Shen, NUS, Singapore	Title: 2DMatPedia: An open computational 2D materials database

Session II B – Parallel: Electronic Properties and Computational Design
Session Chair: Prof. Eunsang Kwon, Tohoku University, Japan

11:30 a.m. – 12:00	Hall 4	Invited Lecture 6	Prof. Udo Schwingeschlögl, KAUST, Saudi Arabia	Title: Valleytronics: A materials perspective
12:05p.m. – 12.35 p.m.	Hall 4	Invited Lecture 7	Prof. Amrita Bhattacharya, IIT Bombay, India	Title: Band engineering to enhance the thermoelectric figure of merit in half-Heusler alloys
12:40 a.m. – 01:10 p.m.	Hall 4	Invited Lecture 8	Prof. Swapan K. Ghosh, University of Mumbai, India	Title: Density functional theory in parameter space: A versatile tool for the investigation of dynamics of many-particle systems.

FRACTMEET 2020
Session II C – Parallel
Session Chair: Prof. Bikas K. Chakrabarti

11.30 a.m. – 12.15 a.m.	Hall-1, 3rd floor	Invited Lecture 9	Prof. Takahiro Hatano, Osaka University, Japan	Title: Complexity of Earthquake Time Series as Probed by Visibility Graph
12.20 a.m. – 01:05 p.m.	Hall-1, 3rd floor	Invited Lecture 10	Prof. Anuradha Banerjee, IIT Madras, India	Title: Micro-structural Aspects and Crushing Response of Bone

01. 10 p.m. – 2.00 p.m.: Lunch Break

Afternoon Sessions

Session IIIA – Parallel: Machine Learning for Materials - I
Session Chair: Prof. K. R. Lee

2.00 p.m. – 2.30 p.m.	Hall 3	Invited Lecture 11	Prof. Saurabh Ghosh, SRMIST, India	Title: Design of functional oxides guided by first-principles calculations and machine learning
2.35 p.m. – 3:05 p.m.	Hall 3	Invited Lecture 12	Prof. Hiroshi Mizuseki, KIST,	Title: Machine Learning on Band

			South Korea	Gap Prediction of III-V Compound Semiconductor
3.10 p.m. – 3.40 p.m.	Hall 3	Invited Lecture 13	Prof. A. K. Singh, IISc, India	Title: Combined High-Throughput and Machine learning Approach for Prediction of Lattice Thermal Conductivity
3:40 p.m. – 4:00 p.m.	Tea/Coffee Break 20 mints			

Session IIIB – Parallel: Energy Materials
Session Chair: Prof. G.P. Das, IIT KGP, India

2.00 p.m. – 2.30 p.m.	Hall 4	Invited Lecture 14	Prof. Saswata Bhattacharya, IIT Delhi, India	Title: Role of defects in MAPbI3 to modulate optical absorption, and solar efficiency
2.35 p.m. – 3:05 p.m.	Hall 4	Invited Lecture 15	Prof. Prasenjit Ghosh, IISER Pune, India	Title: Theoretical investigations of a platinum–water interface using quantum-mechanics-molecular-mechanics based molecular dynamics simulations
3.10 p.m. – 3.40 p.m.	Hall 4	Invited Lecture 16	Prof. Prasenjit Sen, HRI, India	Title: New insights into old materials: Layered ternary tri-chalcogenides and Co-based clusters
3:40 p.m. – 4:00 p.m.	Tea/Coffee Break 20 mints			

FRACTMEET 2020
Session IIIC - Parallel
Session Chair: Prof. Pinaki Chaudhuri

2.00 p.m. – 2.45 p.m.	Hall-1, 3rd floor	Invited Lecture 17	Prof. Lucas Goehring, Nottingham Trent University, UK	Title: Cohesive granular media
2.50 p.m. – 3:35 p.m.	Hall-1, 3rd floor	Invited Lecture 18	Prof. Arghya Das, IIT Kanpur, India	Title: Modelling and simulation of

				confined comminution in crushable granular materials
3:40 p.m. – 4:00 p.m.	Tea/Coffee Break 20 mints			

Session IVA – Parallel: Machine Learning for Materials - II
Session Chair: Prof. Puru Jena, VCU, USA

4.00 p.m. – 4.30 p.m.	Hall 3	Invited Lecture 19	Prof. Nguyen, Duc M, CCFE, UK	Title: First-principles modelling of radiation induced segregation in multi-component systems: From defective Hamiltonian to machine-leaning based smart energy model
4:35 p.m. – 5:05 p.m.	Hall 3	Invited Lectures 20	Dr. DLVK Prasad, IIT Kanpur, India	Title: An MGI approach to free energy landscape of compositional alloys

Session IVB – Parallel: Energy
Session Chair: Prof. Shiv Khanna, VCU, USA

4.00 p.m. – 4.30 p.m.	Hall 4	Invited Lecture 21	Prof. Eunsang Kwon, Tohoku University, Japan	Title: Crystal Structure and Application of Lithium-Cation Endohedral [C60] Fullerene
4:35 p.m. – 4.55 p.m.	Hall 4	YRP1	M.V.M Jyothirmai, SRM IST	Title: Searching of suitable cationic dopants for CZTS/Se using First-Principles study

5:00 p.m. – 5.20 p.m.	Hall 4	YRP2	Dr. Paramita Banerjee, JNCASR, India	Title: Exploring the Efficiency of Carbon Nanostructures for Hydrogen Storage and Oxygen Reduction Reaction

FRACTMEET 2020
Session IVC - Parallel
Session Chair: Prof. Takahiro Hatano

4.00 p.m. – 4:45p.m.	Hall-1, 3rd floor	Invited Lecture 22	Prof. R. Rajesh, IMSc, India	Title: Shock propagation in a dilute medium
4:50 p.m. – 5.15 p.m.	Hall-1, 3rd floor	YRP 3	Dr. Chandreyee Roy, IMSc, Chennai, India	Title: Brittle to quasi-brittle transition in a compound fiber bundle

Buses will start at 5:30 p.m to Hotels

7.30 p.m. – 9.30 p.m.: Dinner for Participants in the venue and Speakers in the Hotels

6th February, Thursday 2020

Venue: Hall 3 and Hall 4, 4th Floor and, Hall 1, 3rd Floor, Admin Block

Session VI
Morning Session: 9.00 a.m. – 1.00 p.m.
Session Chair: Prof. Yoshiyuki Kawazoe, Tohoku University, Japan

9.30 a.m. – 10:00 a.m.	Hall 3	Invited Lecture 23	Prof. Ferenc Kun	Title: Discrete element modelling of the compressive failure of porous rocks
10:05 a.m. – 10.35 a.m.	Hall 3	Invited Lecture 24	Prof. Shiv Khanna, VCU, USA	Title: Transforming Redox Properties of Clusters Using Ligands to Create Super Dopants for Two-Dimensional Semiconductors

				and to Synthesize Nano p-n-junctions
10.35 a.m. – 10:50 a.m.	Tea/Coffee Break 15 mints			

Session VII-A Parallel: Catalyst and Descriptor
Session Chair: Prof. Ranjit Thapa, SRM University - AP

10.50 a.m. – 11:20 a.m.	Hall 3	Invited Lecture 25	Prof. Shobhana Narasimhan, JNCASR, India	Title: Simple Yet Successful Descriptors for Self-Assembly on Surfaces
11.25 p.m. – 11:55 p.m.	Hall 3	Invited Lecture 26	Prof. Hisato Yasumatsu, Tokyo Tech. Japan	Title: Low-temperature and highly-selective catalysis of NO reduction and CO oxidation on platinum cluster disk bound to silicon substrate
12.00 p.m. – 12.30 p.m.	Hall 3	Invited Lecture 27	Prof. Nurbosyn U. Zhanpeisov, Tohoku University, Japan	Title: Theoretical DFT Study on Modified Oxides and Gold Structures
12:35 p.m. – 01:05 p.m.	Hall 3	Invited Lecture 28	Prof. M. Ali Haider, IIT Delhi, India	Title: Rational Catalyst Design Augmented with DFT, Machine Learning and Ab-Initio Microkinetic Modeling

Session VII-B Parallel: Metal oxides, Perovskites and Magnetic Materials
Session Chair: Prof. Nurbosyn U. Zhanpeisov, Tohoku University, Japan

10.50 a.m. – 11:20 a.m.	Hall 4	Invited Lecture 29	Prof. Kersti Hermansson, Uppsala University, Sweden	Title: e-Chemistry of metal oxides – molecule interfaces: data or insights?
11.25 p.m. – 11:55 p.m.	Hall 4	Invited Lecture 30	Prof. B. R. K. Nanada, IIT Madras	Title: Recreating Metal out of Insulators and Insulators out of Metals in Oxide Heterostructures

12.00 p.m. – 12.30 p.m.	Hall 4	Invited Lecture 31	Prof. Subodh Kumar De, IACS, India	Title: Magnetic Properties of Nd_2CoIrO_6 Double Perovskite
12:35 p.m. – 01:05 p.m.	Hall 4	Invited Lecture 32	Prof. Hena Das, Tokyo Institute of Technology, Japan	Title: Exploring the potential of Quadruple perovskites for fast lithium-ion transport

FRACTMEET 2020
Session VII-C Parallel
Session Chair: Prof. Purusattam Ray

11:00 a.m. – 11:45 a.m.	Hall-1, 3rd floor	Invited Lecture 33	Prof. Sujata Tarafdar, Jadavpur University, India	Title: An Interesting Application of Desiccation Crack Networks in Technology
11:50 a.m. – 12:35 p.m.	Hall-1, 3rd floor	Invited Lecture 34	Prof. Akio Nakahara, Nihon University, Japan	Title: Controlled crack patterns produced by memory effect of paste
12:40 p.m. – 13:05 p.m	Hall-1, 3rd floor	YRP4	Dr. Subhadeep Roy, NTNU, Norway	Title: Effective rheology of two-phase flow in porous media: dependence on system disorder

01. 05 p.m. – 2.10 p.m.: Lunch Break

Session VIII-A Parallel: Materials Informatics and Storage
Session Chair: Prof. Ryo Maezono, JAIST , Japan

2.10 p.m. – 2.40 p.m.	Hall 3	Invited Lecture 35	Prof. Kenta Hongo, JAIST, Japan	Title: Computational materials design from materials simulations to

				informatics
2.45 p.m. – 3:05 p.m.	Hall 3	YRP5	Dr. Mudit Dixit, LPU, India	Title: Elucidating the origin of capacity fading of Ni-rich layered oxide-based positive electrode materials for Li-ion batteries
3.10 p.m. – 3.30 p.m.	Hall 3	YRP6	Dr. Aaditya Manjanath, Academia Sinica, Taiwan	Title: Excitation energies from thermally-assisted-occupation density functional theory: Theory and computational implementation
3:35 p.m. – 3:45 p.m.	Hall 3	Oral1	Dr. Tong Yang, NUS, Singapore	Title: High-Throughput Screening Of Single Transition Metal Atoms Anchored On Mos2 Monolayer For Nitrogen Fixation

Session VIII-B Parallel
Session Chair: Prof. Nguyen, Duc M, Culham Centre for Fusion Energy, UK

2.10 p.m. – 2.40 p.m.	Hall 4	Invited Lecture 36	Dr. Mahesh Kumar Ravva, SRM-AP	Title: Theoretical design and development of new macrocycle organic materials for organic electronic applications
2.45 p.m. – 3:15 p.m.	Hall 4	Invited Lecture 37	Prof. Vannajan Sanghiran Lee, University of Malaya, Malaysia	Title: Quasiparticle energies of ground state and excited state of metal clusters using all-electron mixed basis of plane waves (PWs) and atomic

				orbitals (AOs)
3:15 p.m – 3: 45 p.m	Hall 4	Invited Lecture 38	Prof. V. Subramanian, CLRI, India	Title: Computational Evaluation of Donor-Bridge-Acceptor (D-B-A) Motifs for High Performance Optoelectronic Device Applications
3.45 p.m. – 4:.05 p.m.	Hall 4	YRP7	Dr. Kanchan Ulman, NUS, Singapore	Title: Understanding the chemical enhancement mechanism of 2D substrate enhanced Raman Spectroscopy (2D-SERS)

FRACTMEET 2020
Session VIII-C Parallel
Session Chair: Prof. Sujata Tarafdar

2.10 p.m. – 2.55 p.m.	Hall-1, 3rd floor	Invited Lecture 39	Prof. Parag Tandaiya, IIT Bombay, India	Title: Mechanics and Mechanisms of Deformation and Failure in Heterogeneous Amorphous Alloys: Insights from Continuum Simulations of Porous BMGs and ex-situ BMG Composites
3.00 p.m. – 3:25 p.m.	Hall-1, 3rd floor	YRP8	Prof. Srutarshi Pradhan, NTNU, Norway	Predicting the collapse point of materials under stress
3:30p.m.-4:15p.m.	Hall-1, 3rd floor	Invited lecture 40	Prof. Bikas K. Chakrabarti, SINP, India	Title: Kolmogorov Dispersion for Turbulence & Statistics of Fracture in the Fiber Bundle Model

Evening Session: 4.00 p.m. – 6.00 p.m.: Poster session with Tea/coffee
Venue: Atrium

7.30 p.m. – 9.30 p.m.: Banquet Dinner
Bus will start at 6:30 P.M to venue for Banquet Dinner, Please wear the conference ID card

7th February, Friday 2020

Morning Session: 9.00 a.m. – 1.00 p.m.
Session IX a
Session Chair: Prof. Jungsuttiwong Siriporn

9.30 a.m. – 10.00 a.m.	Hall 3	Invited Lecture 41	Prof. Ranjit Thapa, SRM-AP	Title: Electronic Descriptor for carbon catalyst using QM/ML approach
10:05 a.m – 10:35 a.m	Hall 3	Invited Lecture 42	Prof. Ryo Maezono, JAIST, Japan	Title: Ab initio Quantum Monte Carlo method; Role in Materials Genome
10.35 a.m. – 10.50 a.m.	Tea/Coffee Break 15 mints			

Session X-A Parallel: Energy, Plasmonic and ML
Session Chair: Prof. Kenta Hongo

10.50 a.m. – 11:20 a.m.	Hall 3	Invited Lecture 43	Prof. Tanmay Basak, IIT Madras, India	Title: Analysis of heat flow visualization and thermodynamic efficiency during thermal convection in cavities with distributed solar heaters
11.25 a.m. – 11:55 a.m.	Hall 3	Invited Lecture 44	Prof. MAJIDI Muhammad Aziz, Universitas Indonesia	Title: Controlling plasmonic characteristics through confinement and correlation effects
12:00 p.m – 12:10 p.m	Hall 3	Oral 2	Dr. Kavita Joshi, NCL, India	Title: Combining DFT With ML To Study Size Specific Interactions Between Metal Clusters And Adsorbates

12:15 p.m – 12:25 p.m	Hall 3	Oral 3	Mr. Amrish Kumar, IIT Delhi, India	Title: Rational Design Of Single Atom Catalysts Based On Cu, Ag And Au Alloys Using Machine Learning Approaches

Session X-B Parallel: Chemical and Thermal Analysis
Session Chair: Prof.Vannajan Sanghiran Lee

10.50 a.m. – 11:20 a.m.	Hall 4	Invited Lecture 45	Prof. Kothandaraman Ramanujam, IIT Madras, India	Title: Catalysis on the surface of nanotubes having confined solvent media
11:25 p.m. – 11:55 p.m.	Hall 4	Invited Lecture 46	Prof. JUNGSUTTIWONG, Siriporn, URU, Thailand	Title: Theoretical and Mechanistic Studies on Catalysis of Carbon Dioxide Hydrogenation to Formic Acid on Pt doped Boron Nitride Nanosheets
12:00 p.m – 12: 10 p.m	Hall 4	Oral 4	Dr. Sujith Kalluri, SRM University -AP	Title: Thermal analysis of Myristic -Layric acid –Fe2O3 composite as nano-enhanced organic phase change material
12:15 p.m – 12:25 p.m	Hall 4	Oral5	Dr. V. Arivindan, Thiagarajar College of Engineering, India	Title: First Principles Study Of Structural, Electronic, Magnetic And Elastic Properties Of The Mn2-X-Sb (X= Co, Fe) Inverse Heusler Alloys

FRACTMEET 2020
Session X-C Parallel
Session Chair: Prof. Lucas Goehring

11.00 a.m. – 11:45 a.m.	Hall-1, 3rd floor	Invited Lecture 47	Prof. V. Madhurima, Central Uni. Tamil Nadu, India	Title: Lubrication Driven Hierarchical Self-Assembly of Droplets
11.50 p.m. – 12:35 p.m.	Hall-1, 3rd floor	Invited Lecture 48	Prof. Smarajit Karmakar, TIFR Hyderabad, India	Title: Yielding at bulk and Nanoscale amorphous solids
12:40 p.m – 01:25 p.m	Hall-1, 3rd floor	Invited Lecture 49	Prof. Koushik Vishwanathan, IISc Bangalore, India	Title: Stick-slip in soft polymers: Elasticity, adhesion and slow wave propagation

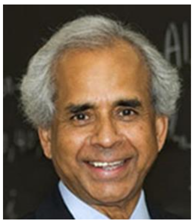
Closing Remarks: 12:45 p.m to 01:15 p.m

Lunch 01:15 to 02:15 p.m.

Half Day Tour 2:30 to 6:00 p.m.
Dinner in the respective accommodation places

Invited Speakers

IL-1: In Search of Metastable Forms of Carbon



Prof. Puru Jena
Virginia Commonwealth University, Richmond

Metastable forms of matter often possess properties superior to those of their ground state. A case in point is diamond *vs*. graphite. Yet, in practice, many predicted metastable structures are dismissed as hard-to-realize. We introduce a method that can enhance the realizability of a targeted metastable structure against the ground state in the potential energy surface and directly guide its experimental synthesis. This is done by selecting a proper precursor according to the building block of the targeted structure and forming topological assemblies of the precursor molecules. The method is applied to realize metastable forms of carbon, which is one of the most fascinating elements in the periodic table. The unique properties of carbon emerge from its ability to form diverse sp^n ($1 < n < 3$) bonds, graphite with sp^2 and diamond with sp^3 bonding being the most common forms. The discovery of zero-dimensional (0D) carbon fullerenes, one-dimensional (1D) chain-like carbyne and carbon nanotube, and two-dimensional (2D) graphene, all with novel properties characteristic of their reduced dimensionality and size, has ushered a new era in carbon science. In recent years many new metastable forms of carbon exhibiting a mixture sp^1, sp^2 and/or sp^3 bonding pattern have also emerged. In this talk I will focus on the carbon allotropes that have been studied in our group[1-6]. These include functionalized C_{60} fullerenes for hydrogen storage[1,2], semi-hydrogenated graphene for metal-free ferromagnet[3], 3D metallic carbon made of hybridized sp^2 and sp^3 bonded atoms[4], and a Cairo-tilling inspired quasi-2D penta-graphene made only of carbon pentagons[5]. I will highlight the discovery[6] of a new carbon allotrope, named U-carbon, that is composed of carbon atoms forming both sp^2 and sp^3 bonds. Arranged in four- and six-membered rings, U-carbon is metallic and magnetic. Theoretical studies were carried out using a multi-scale first-principles approach while experiment was conducted using chemical vapor deposition of the targeted organic precursor molecule. Potential applications of some of these carbon allotropes will be discussed.

IL-2: Theoretical Materials Research in Past and Future

Prof. Yoshiyuki Kawazoe, Tohoku University, Japan

Starting from alchemy, it has been a long dream for human to create new useful (expensive) materials from common (cheap) atoms. After the modern chemistry established, it is now clear to know that it is not possible (too much energy is necessary and not cost effective) to change nuclear species (cheap metal to gold). On the contrary we can create new useful molecules and crystals from common elements; even organic molecules are synthesized from inorganic things. After 150 years of the periodic table by Mendelejev, we now can design new materials selecting from the table, and composing new useful materials in reality. In last year there was a big change in all science and engineering; the new definition of metrics by atomic units changed from MKSA system used for 200 years. It is very good for us, since we have been used to use the atomic units in our equations all the time. There have been two big users of supercomputing systems in the history; computational fluid dynamics (CFD) and computational materials science (CMS). CFD has more than 200 years of history, but CMS has less than 60 years after Prof. Kohn's density functional theory (DFT) in 1964. After Dr. Dongarra started his report in 1993, computer power has continuously grown 10 times/5 years (Moore's law); actually 100,000 times faster after that! Based on this computing power, we have been developing and applying our simulation software in two ways; (1) add better approximations for more realistic calculations, and (2) increasing the number of atoms, even protein are the targets now. Recent most important change in CMS is to work with artificial intelligence (AI) named materials informatics (MI), where we compute throughout the periodic table and generate big data and apply backward prediction strategy to find out the new materials with requested properties. To do this aim, really a large number of possible systems (normally more than 10,000 cases) are computed with DFT, which is possible only based on the available large computing power. However, still a fundamental problem remains, which is the present problem of "no improvement in clock speed for over 10 years". Basically the speed-up of the supercomputer is realized by the increase of number of cores (similarly CPUs and nodes), and one core (CPU, node) is good enough for one DFT calculation, and therefore a large number of DFT computing is possible. However, for example, predict new materials which emits specific color (for example green color LED), it is minimum to apply GW calculation, which is still costly and not possible to compute 10,000 cases. At the moment, we computer simulation people can't do similarly good as experimentalists, but in our future based on the Moore's law is kept, we can reach and enjoy "Theory First" situation in CMS based on our rule (quantum mechanics), which has been the standard in elementary particle physics.

IL-3: Computational design of low dimensional materials for energy applications

Prof. G.P. Das
Indian Institute of Technology Kharagpur, Kharagpur

In this talk, I shall start with an overview of the essential materials requirements for storage of renewable energies. I shall then focus on some nanostructures, in particular carbon based nanostructures, that are candidate materials for efficient storage of hydrogen and also as metal-free catalysts for water splitting and low temperature fuel cells. First principles density functional based simulation prove extremely handy in designing such novel materials with desired combination of properties. After presenting some case studies that are mostly on functionalized 2D materials [1-6], I shall wrap up by discussing how the advent of materials informatics is expanding the horizons of the computational design of low dimensional materials.

IL-4: SimPL: A Framework for Web-based Materials Design Platform

Prof. Kwang-Ryeol Lee
Korea Institute of Science and Technology, Seoul, Korea

Owing to the rapid increase in computing power and successful advancement of the computation methods, (sub) atomic simulation has been driven new paradigm of materials research. However, the high entrance barrier against the computational materials research need to be further reduced for wider application of the (sub)atomic materials simulation techniques. Our group has been developing thematics simulation platforms: virtual fab of nano materials (http://nano.vfab.org) and battery materials design platform (http://battery.vfab.org). These platforms provide the working environment where one can perform advanced computational research according to the workflow of familiar experimental research. Based on our experience with the thematic multiscale simulation platforms, we developed the framework for providing modules of various functions that are essential for the web-based simulation platforms. The framework, named as “SimPL”, is composed of pages and functional plug-ins that can make it easy to build any thematic simulation platform of user’s needs. In this poster, we will introduce the SimPL framework and share the access information in www.vfab.org. We will also present the application cases using SimPL and discuss it’s application for data-driven materials research.

IL-5: 2DMatPedia: An open computational 2D materials database

Prof. Lei Shen
National University of Singapore, Singapore

Two-dimensional (2D) materials have been a hot research topic in the last decade, due to novel fundamental physics in the reduced dimension and appealing applications. Thus, it is important and timely to systematically discover new functional 2D materials for potential various applications. On behalf of our team, here, I will introduce our recent work on the world largest 2D materials database (http://www.2dmatpedia.org/) and its applications via several examples. In the first part, I will be talking about how we screen out more than 6,000 2D materials through the high-throughput calculations and materials genome. The structural, electronic and energetic properties of these 2D materials are consistently calculated, to provide a starting point for further material screening, data mining, data analysis and artificial intelligence applications. The details of computational methodology, data record and technical validation of our publicly available data are presented in http://www.2dmatpedia.org/ and https://www.nature.com/articles/s41597-019-0097-3). In the second part, I will brief several examples of applications utilizing 2D materials database, including 1) searching high-performance flexible solar cells, 2) exploring high-temperature 2D ferromagnets, 3) data-mining exotic 2D electrides, 4) machine and/or deep learning physical properties of 2D materials.

IL-6: Valleytronics: A materials perspective

Prof. Udo Schwingeschlögl
King Abdullah University of Science and Technology, Saudi Arabia

Silicene and germanene are key materials for the field of valleytronics. However, interaction with the substrate, which is necessary to support the electronically active medium, becomes a major obstacle. We show that magnetically doped WS2 can be used as substrate that avoids detrimental effects and at the same time induces valley polarization. Broken inversion symmetry due to the presence of WS2 opens a substantial band gap in silicene and germanene, and the induced spin polarization in conjunction with proximity-enhanced spin-orbit coupling creates sizable valley polarization. We also discuss the possibility to generate valley polarization in 2D MoS2 by substitutional magnetic doping. An unprecedented physical-chemical mechanism, based on delicate interplay between defect state and extended moment formation, is identified as source of the valley polarization.

IL-7: Band engineering to enhance the thermoelectric figure of merit in half-Heusler alloys

Prof. Amrita Bhattacharya
IIT Bombay, India

Thermoelectrics can be a viable alternative to a green energy economy via waste heat recovery given that more than 60% of the produced energy is lost in the form of waste heat worldwide [1]. The dimensionless figure-of-merit ($ZT = TS2\sigma/\kappa$, Seebeck coefficient (S), electrical conductivity (σ), thermal conductivity (κ) and T is the absolute temperature) drives the thermoelectric efficiency. Half-Heusler (HH) compounds (XYZ, where X and Y are transition metals and Z is a main group element) have emerged as promising thermoelectric materials that offers huge chemical space with tunable band gap to optimise their thermoelectric performance [2]. Starting with the earth abundant ZrNiSn composition, we explore the pathways to enhance its thermoelectric performance via band engineering by chemical substitution at the different sites with elements from the same group. For this purpose, we employ density functional theory calculations to explore the stability, electronic structure and transport properties of XpX’1-pYqY’1-qZrZ’1-r (X, X’ = Ti, Zr, Hf; Y, Y’ = Ni, Pd, Pt and Z, Z’ = Ge, Sn, Pb) compositions, where p, q, and r are the different concentration of elemental substitution at the X, Y and Z sites respectively. For this purpose, we calculate the formation energy of all the parent compounds as well as the different solid solutions. Our calculations show that all these Heusler compounds are stable with negative formation energy with their band gap in the range of 0.4 -1.0 eV. Earlier reports suggested that Hf0.5Zr0.5NiSn to be the one with highest power factor. Our results are in confirmation of this. However, we suggest an alternative path to achieve a higher power factor (S2σ) without alloying with Hf, since the cost effective deployment of Hf based thermoelectric is nontrivial. We calculate the transport coefficients of the compounds using semiclassical Boltzmann transport theory. Furthermore, we calculate the Gruneisen parameter and group velocity by employing harmonic vibrational calculations. Our preliminary calculations suggest that substitution with Ge on the Z site is a possible solution to realise Hf free thermoelectric compound, which has a comparable power factor but low lattice thermal conductivity.

IL-8: Density functional theory in parameter space: A versatile tool for the investigation of dynamics of many-particle systems

Prof. Swapan K. Ghosh
UM-DAE-Centre for Excellence in Basic Sciences, University of Mumbai

Density functional theory (DFT) has been a versatile tool for the quantum mechanical description of atoms, molecules and solids using electron density as the basic variable. It has also been extended to the classical domain in terms of the particle number density within the framework of statistical mechanics. The scope of DFT is further broadened to encompass a parameter space density variable, which has applicability to a wide variety of dynamical phenomena involving many-particle systems in condensed phase covering diverse areas of research in chemistry, physics, biology and related disciplines. We first discuss here the theoretical formalism for the development of a novel unified parameter space DFT by considering a reduced space description through projection of the fundamental Liouville equation to a general phase space function or reaction coordinate space, following closely the pioneering work of Zwanzig and its extensions. We then consider the various conceptual aspects associated with the approach and application to the structure and dynamics in condensed phase, in particular photo-induced solvation dynamics and electron transfer reactions [4-5]. The new approach is shown to take into account the effect of not only the thermodynamic parameters but also the photo-excitation wavelength on the dynamics of the non-equilibrium processes in condensed phase, in consistency with experimental observations.

IL-9: Complexity of Earthquake Time Series as Probed by Visibility Graph

Prof. Takahiro Hatano

Department of Earth and Space Science, Osaka University, Osaka, Japan

In this talk, we present a novel approach to earthquake statistics based on a network theory. Here a network is actually a (mathematical) graph that consists of the points (referred to as “nodes”) and the lines that connect points (referred to as “edges”). In conventional studies on seismicity, earthquakes are regarded as points in the space-time. Thus, one can construct a graph by regarding each earthquake as a node, connecting two earthquakes according to an appropriate rule. On the other hand, the nodes are not necessarily earthquakes. For instance, a node can be a mesh in the space-time, where an earthquake occurs. Here we introduce two different methods to construct a graph from earthquake catalogs: (i) Visibility graph in the time-domain and (ii) Connecting two meshes where two consecutive earthquakes occur. We show that a visibility graph possesses some intriguing properties such as “small-world”. The graph can also show that the magnitudes of earthquakes are uncorrelated in the time domain, supporting a key assumption made in the ETAS models. We also show that type ii graph can reveal essential differences between fast and slow earthquakes.

Keywords: visibility graph; earthquake; complex network

IL-10: Micro-structural Aspects and Crushing Response of Bone

Prof. Anuradha Banerjee
IIT Madras

Cortical bone material, found in mechanical load bearing bones like femur, is known to have two distinct microstructures. In this talk, I will present our findings on the individual roles of the mean porosity, structure of the network of pores and bone matrix properties in the fracture behavior of these two types of bone microstructures. We first determine the detailed structure of porosity network both pre- and post-testing of cubical bone samples using micro- omputed Tomography. Based on the periodicity in the features of porosity, we develop a two dimensional porosity- based random spring network model. The model is shown to capture well the macroscopic response and reproduce the avalanche statistics similar to recently reported experiments on porcine bone. The predictions suggest that at the millimeter scale, the remodeled bone matrix of Haversian bone is less stiff but tougher than that of plexiform/primary bone.

IL-11: Design of functional oxides guided by first-principles calculation and machine learning

Prof. Saurabh Ghosh
SRM Institute of Science and Technology, Kattankulathur

The Density Functional Theory (DFT), which is a first principles method, has been the governing method for quantum mechanical simulation of materials for the past 30 years. Using this theory structural, electronic, magnetic and other properties of a many electron system can be determined. With the advancement of modern supercomputing capabilities, DFT is not only successful in explaining experimental findings but also predicting materials with new functionalities. On the other hand, Machine Learning (ML) refers to the automated detection of meaningful patterns in the data. It is a common tool to use in a task which requires information extraction from a large data set. The ML based algorithms are used in search engines, in credit card transitions, digital camera, flight scheduling and many more, in almost every accepts of our modern-day life. In this regard the application of ML and artificial intelligence (AI) based approach is rather new in materials science. The ML and AN based approach can be used to predict new materials for enhanced functionality or to make strategies to enhance a particular property of a particular material. In the context of designing new materials, understanding the ‘structure-property’ relationship of a material is the key. In this talk I will discuss ‘structure-property’ relation of functional materials based on DFT calculations and machine learning and by considering ABO3 perovskite oxide heterostructures as prototype examples [1-3]. The focus will be given on functional oxide materials that can impact energy, electronics and spintronics industry.

IL-12: Machine Learning on Band Gap Prediction of III-V Compound Semiconductor

Prof. Hiroshi Mizuseki
Korea Institute of Science and Technology (KIST), Seoul, Republic of Korea

III-V alloy is a typical semiconductor, containing elements from groups III and V in the periodic table. The materials obtained from these elements provide a new way to tune the electronic properties by natural means and widen their potential applications especially in optoelectronic devices. Moreover, by controlling the alloy composition, a desired band gap in principle can be obtained for specific application purpose. However, it is challenging to handle the large set of alloy combinations and predict the desired band gap. Therefore, a prediction technique is essential to address this important issue. It is well known that GW-method can be used to obtain an accurate band gap. However, this approach becomes computationally expensive to handle the large number of alloy combinations. In the present study, we apply machine learning approach such as neural network for PBE-level band gap to predict band gap values of III-V compounds over a wide range of compositions. Here we also investigate the relative stability between zincblende and wurtzite structures as well as other material properties.

IL-13: Combined High-Throughput and Machine Learning Approach for Prediction of Lattice Thermal Conductivity

Prof. Abhishek K. Singh
Materials Research Centre, Indian Institute of Science, Bangalore

Lattice thermal conductivity κl is very important material property. While low κl materials are crucial for applications such as the thermoelectric conversion of waste heat to useful energy and thermal barrier coatings, high κl materials are necessary for cooling electronic devices. However, search for such materials via explicit evaluation of κl either experimentally or computationally is very challenging. Here, we carried out high-throughput ab initio calculations, on a dataset containing 195 binary, ternary, and quaternary compounds. The κl values of 120 dynamically stable and nonmetallic compounds are calculated, which span over 3 orders of magnitude. Among these, 11 ultrahigh and 15 ultralow κl materials are identified. An analysis of generated property map of this dataset reveals a strong dependence of κl on simple descriptors, namely, maximum phonon frequency, integrated Grüneisen parameter up to 3 THz, average atomic mass, and volume of the unit cell. Using these descriptors, a Gaussian process regression-based machine learning (ML) model is developed. The model predicts room temperature log-scaled κl with a very small root mean square error of ∼0.21. As the quasi-harmonic properties also appear in the Slack model, which is a very popular physics-based model for the prediction of κl, we employed it on our dataset for the comparison. The Slack model severely overestimates κl, highlighting the exceptional performance of the developed machine learning model. The superior performance of the ML model can ensure a reliable and accelerated search for a multitude of low and high thermal conductivity materials.

IL-14: Title: Role of defects in MAPbI3 to modulate optical absorption, and solar efficiency

Prof. Saswata Bhattacharya
IIT Delhi, India

We address the role of Sn-substitution and Pb-vacancy (Pb-⊠) in reducing the Pb concentration and enhancing the stability of mixed perovskite CH3NH3Pb1-X-YSnX⊠YI3 using state-of-the-art hybrid density functional theory. The role of spin orbit coupling (SOC) and electron self-interaction error are examined carefully. Despite SOC has a significant role in artificially shifting the electronic bands, it doesn't affect the relative hierarchy of formation energies of different defected configurations. However, electron self-interaction plays an important role in determining the same. We find a semi-local functional (e.g. PBE) gives completely opposite trend to determine thermodynamic stability w.r.t HSE06+SOC. We obtain, to reduce the Pb-content from pristine MAPbI3, Sn-substitution has a favorable thermodynamic stability than Pb-⊠. This has been inferred from the lower formation energy of (charged) Sn substitution in the Pb8I24 framework as compared to a (charged) Pb-⊠ vacancy creation. For n-type and p-type host, the Sn substitution is more preferable than Pb-⊠ formation. Further, the optical properties and spectroscopic limited maximum efficiency (SLME) for thermodynamically stable configurations (Sn-substitutions) are also calculated. We have achieved highest efficiency of 33% for MA8Pb7Sn1I24, and for other cases upto 50% Sn, the efficiency is reasonably good as compared to pristine. The stability of the doped perovskites are also confirmed at higher temperatures using ab initio Molecular Dynamics (AIMD) simulation. The lower formation energy, structural stability, direct p-p/s-p transition, high optical absorption coefficient (red shifted), stability at operational temperature and maximum solar cell efficiency of the CH3NH3Pb1−XSnXI3 ($0 \leq X \leq 0.5$) makes it a promising candidate for highly efficient solar cell absorber.

IL-15: Theoretical investigations of a platinum–water interface using quantum-mechanics-molecular-mechanics based molecular dynamics simulations

Prof. Prasenjit Ghosh
IISER Pune, India

Pt–water interfaces have been of immense interest in the field of energy storage and conversion. Studying this interface using both experimental and theoretical tools is challenging. On the theoretical front, typically one uses classical molecular dynamics (MD) simulations to handle large system sizes or time scales while for a more accurate quantum mechanical description Born Oppenheimer MD (BOMD) is typically used. The latter is limited to smaller system sizes and time-scales. In this study using quantum-mechanics-molecular-mechanics (QMMM), we have performed atomistic MD simulations to have a microscopic understanding of the structure of the Pt–water interface using a system size that is much larger than that accessible when using BOMD simulations. In contrast to recent reports using BOMD simulations, our study reveals that the water molecules typically form two distinct layers above the Pt-surface before they form bulk like structures. Further, we also find that a significant fraction of the water molecules at the interface are pointed towards the surface thereby disrupting the H-bond network. Consistent with this observation, the layer resolved oxygen–oxygen radial distribution function for the water molecules belonging to the solvating water layer shows a high density liquid like behaviour even though the overall water behaves like a low density liquid. A charge transfer analysis reveals that this solvating water layer donates electrons to the Pt atoms in contact with it thereby resulting in the formation of an interface dipole that is pointing towards the surface. Our results suggest that, using QMMM-MD, on one hand it is possible to study more realistic models of solid–liquid interfaces that are inaccessible with BOMD, while on the other hand one also has access to information about such systems that are not obtained from conventional classical MD simulations.

IL-16: New insights into old materials: Layered ternary tri-chalcogenides and Co-based clusters

Prof. Prasenjit Sen,
HRI, India

Layered ternary transition metal (TM) tri-chalcogenides with the general formula MAX3 (M=TM; A=Si, Ge or P; and X=chalcogen) have been known and characterized extensively for decades. Most of them are magnetic semiconductors, generating interest in their fundamental properties, They also have potential for various applications. With the current interest in 2D materials, exploration of these compounds has received a new lease of life. Some of these compounds have shown interesting magnetic transitions in two dimensions, and promising catalytic behavior in hydrogen evolution (HER) and oxygen evolution reactions (OER). We have developed new insights into the electronic structure of some of the Mn and Fe based tri-chalcogenide compounds. In particular, we have been able to correctly describe the ground state of FePSe3, which some earlier works failed to do. We have also explored a number of such compounds, both known and unknown, for their efficiency in HER. The second part of my talk will be on cobalt-based clusters. Some Co-carbide nano-particles have shown unexpectedly large magnetic anisotropy energy (MAE), making them interesting candidates for permanent magnets without rare earth elements. However, a microscopic analysis of the factors determining MAE in these systems was lacking. We have tried to arrive at an easily computable predictor that determines MAE in Co4A2 clusters (A= group 14 or 15 elements), and possibly in other Co-based nano-materials.

IL-17: Cohesive granular media

Prof. Lucas Goehring
School of Science and Technology, Nottingham Trent University, UK

A wide range of solid, porous materials, such as sandstone, concrete and snow, can be accurately described as rigid particles with sticky, sintered or cohesive contacts. Here, we consider the general behavior of such cohesive granular media, and how they fail. We have recently developed a simple experimental realization of a cohesive granular material, consisting of glass beads bound together by narrow polymer (PDMS) bridges, which has tunable properties including its elasticity, fracture toughness, and permeability. In this talk I will describe and characterize this material and show how its macroscopic properties follow from the microscopic constitutive laws linking adjacent particles. Surprisingly, almost all of the material's response to strain is determined by the bonds between particles, which can be as little as ~1% of the volume of the solid structure. I will also detail our minimal model of these materials, which is fully constrained by experimental measurements and which has good predictive power. Under simple compression, this model shows a smooth transition from shear banding, to plastic deformation, to compaction banding, as porosity increases.

Keywords: fracture, failure, granular media, tomography, simulation

IL-18: Modelling and simulation of confined comminution in crushable granular materials

Prof. Arghya Das,
Department of Civil Engineering, IIT Kanpur, UP

Particle crushing in granular materials, in the form of either attrition or comminution, is a complex deformation mechanism that alters the inherent properties of the original granular assembly. Consequently, the macroscopic properties of the granular material, stiffness, and strain hardening response vary, which are the prime objectives for the development of any continuum-based constitutive model. However, prior to the modelling of those macroscopic events, several micromechanical aspects associated with particle crushing like fracture propagation through the grains, creation of new surface area, energy associated with crushing dissipation, and post crushing energy redistribution process need to be understood. In the present study, a micromechanical analysis is carried out using discrete element modelling (DEM) to explore the effects of 1) variation in the loading rates, within/near the quasi-static regime, on the stress-strain response of crushable and non-crushable granular assemblies, and 2) evolution of particle shape during crushing. The simulation shows that the variation in the contact force distribution within the granular assembly at different loading rates dictates the stress response and the crushing events. Relatively low strain rate compression favors homogeneous crushing involving a large number of particles that consequently reduces the strength via fragments rearrangement. Conversely, a high strain rate promotes localized crushing within fewer particles, and thus strain hardening is observed. The analysis of particle shape evolution indicates an increase in the contact anisotropy at the intermediate stages of crushing. However, such effect diminishes with prolonged crushing and fines creation.

IL-19: First-principles modelling of radiation induced segregation in multi-component systems: From defective Hamiltonian to machine-leaning based smart energy model

Prof. Nguyen, Duc M.
CCFE, UK

Understanding the origin of radiation induced segregation (RIS) in materials under neutron irradiation is a phenomenon that has significant practical implications in fusion devices. Recent experimental observations showed a strong presence of RIS in form voids decorated with Rhenium and Osmium transmutation products in neutron-irradiated Tungsten samples. In this talk, a new constrained Hamiltonian approach, based on first-principles calculations, is developed, where solute atoms (Re, Os, Ta) and defects are treated as components of a multi-component alloy system. In the low solute concentration range, our quenched MC predictions for W-1.5%Re-0.1%Os alloys at T=1200K show a strong radiation-induced precipitation with the concentration profiles that can be explained by the dependence of Re-Os negative short-range order parameter as a function of temperature. This finding of anomalous segregation is in an excellent agreement with Atom Probe Tomography and Transmission Electron Microscopy results. To understand the microstructural evolution of the RIS, we extend our Hamiltonian approach to investigate kinetic properties of transmutation products in concentrated W-Re-Os alloys by a smart energy model to characterize the structure of defect clusters via machine-learning algorithm which is inspired to graphs used in biochemistry to predict molecular properties. The consistency between energetic and kinetic models allows us to compute the transport coefficients under varying Re/Os concentrations and to determine how Re and Os drag and segregation to the precipitation with vacancies. It is found that due to Re-Os coupling, appearance of Os in W-Re enhances Re drag to the RIS.

IL-20: An MGI approach to free energy landscape of compositional alloys

Dr. DLVK Prasad
IIT Kanpur, India

Predicting crystal structures for a given composition remains one of the biggest challenges in materials science. In this talk, I will present our recent progress on predicting crystal structures for two types of binary alloy systems via a hybrid materials genome initiative (MGI) approach – a combined global minimum search of free-energy landscape by using first principles evolutionary and knowledge based crystal structure prediction approaches. The methods and results of our investigations will be presented. A case study in the light of superconductivity in Ag-Au fcc binary alloys and an eutectoid decomposition in a catalytically important Fe-Al bcc-fcc solid structures will be discussed.

IL-21: Crystal Structure and Application of Lithium-Cation Endohedral [C60] Fullerene

Prof. Eunsang Kwon,
Tohoku University, Japan

Since the synthesis and characterization of lithium cation endohedral metallofullerene1), Li+@C60 (1), several investigations have been performed on the application of 1 to the functional materials2). The essential structural features of 1 would be as having lithium cation inside the spherical empty space of C60 fullerene. However, due to the low electron density related to the positional and dynamic disorder of the Li+, previous researches faced the limitations of the detailed information of the Li+. In the present work, we investigated the structure of 1 using powder neutron diffraction measurement at low temperature (3.7 K). Moreover, we studied the spectroscopic properties of 1, and their possibility of application to an electrical energy storage system. The scattering length density distributions of the endohedral lithium ions of 1 were successfully obtained from neutron diffraction data using the maximum-entropy method. In addition, the supercapacitor using 1 had a higher charging efficiency and faster charging speed compared with a normal one. Furthermore, we introduce the terahertz and solid-state NMR spectroscopies of 1.

IL-22: Shock propagation in a dilute medium

Prof. R. Rajesh
The Institute of Mathematical Sciences, Chennai

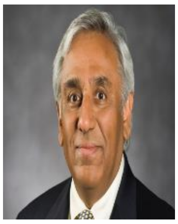
What is the response of a dilute medium, elastic or inelastic, to the input of a large amount of energy in a localised spatial region? A shock wave propagates through the disturbance when the speed of the disturbance exceeds that of the speed of sound. This results in discontinuities in the different thermodynamic quantities across the shock front. In this talk, I will discuss he historical background of this problem including the hydrodynamical approach, describe experiments where the discontinuities may be observed, and the results from simple models that capture the essential features of the problem.

IL-23: Discrete element modelling of the compressive failure of porous rocks

Prof. Ferenc Kun
University of Debrecen, Hungary

Understanding the processes that lead to catastrophic failure of porous granular media is an important problem in a wide variety of applications, notably in Earth science and engineering. Such failure is often preceded by detectable acoustic emissions which may be used to forecast the impending catastrophic event. Under compressive loading in the vicinity of failure localization emerges such that cracking events get concentrated in a damage band where eventually a macroscopic crack develops and the system falls apart. For a comprehensive understanding of the spatial structure of damage and of the statistics and dynamical features of acoustic emissions computer simulation of realistic models is indispensible. We present a discrete element modelling approach of the compressive failure of porous rocks which is able to capture both the intermittent dynamics of fracturing and the complexity of the spatial structure of damage. The model is initiated by filling a cylindrical container with randomly sized spherical particles that are then connected by breakable beams. Simulating the strain controlled uniaxial compression of cylindrical specimens, we demonstrate that the magnitude, energy, and duration of crackling events are characterized by power law distributions. As the fracture process evolves, the magnitude of crackling bursts and the waiting time between consecutive events get correlated. To characterize the approach to failure we analyze the record statistics of the sequence of breaking bursts. We show that the degree of materials’ disorder has a strong effect on the spatial structure of damage which can be described by scaling laws.

IL-24: Transforming Redox Properties of Clusters Using Ligands to Create Super Dopants for Two-Dimensional Semiconductors and to Synthesize Nano p- n- junctions



Prof. Shiv Khanna,
VCU, USA

A promising direction in the research on clusters is to design nanomaterials with size selected clusters or the nanoparticles as the building blocks. Since the properties of clusters/nanoparticles change with size and composition, nano-assemblies offer the unique prospect of designing nanoscale materials with controlled properties. The presentation will focus on using ligands to transform the redox properties of a variety of clusters and their use as dopants to design novel semiconductors where the location of Fermi energy and n- and p- characteristics can be controlled. I will end my talk with a recent discovery where we have used ligands to induce intense electric fields and dipole moments in molecules of homo-atomic clusters. Such units have the characteristics of nano p- n- junctions. Organic ligands that protect the surfaces of clusters and nanoparticles against reactions and control the rate of growth are generally considered to be inert passive coatings. I will demonstrate that the ligands can also strongly affect the redox properties of clusters. I will present our results of the effect of ligation on the ionization energy (I.E). of a variety of clusters including simple and noble metal clusters, Au7, Au11, Au13Cl2, Ag11, and Al7; an Al4O6 cluster corresponding to an insulator; Ga12N12, and Zn12O12 as representative of semiconductor clusters; Co6, Pd6, and Pd7 as representative of transition metal clusters; and Mo6Te8 corresponding to the important metal-chalcogenide clusters recently synthesized by Roy and co-workers. For all cases, the ionization energy is reduced. In many cases, ligated clusters are transformed into super donors with ionization energies nearly half that of cesium atoms, and extremely low second and third ionization energies creating super donors that can donate multiple electrons. I will show that the reduction in ionization energy can be split into initial and final state effects. The initial state effect derives in part from the surface dipole, but primarily through the formation of bonding/antibonding orbitals that shifts the HOMO. The final state effect derives from the enhanced binding of the donor ligand to the charged cluster. The new donor and acceptor superatoms can be used to create doped semiconductors by using superatoms, as effective super-dopants for two-dimensional semiconducting films. Unlike conventional dopants that are embedded in the semiconductor, the superatom dopants act by using the two dimensional semiconductor as a solid state ligand. I will demonstrate this intriguing possibility by considering WSe2 films that are transformed from a p-type to an n-type semiconductor when Co6Se8(PEt3)6 (PEt3- tri-ethylphosphene) superatoms are supported on the surface. The theoretical findings complement recent experiments by Yu et. al. where WSe2 films doped with Co6Se8(PEt3)6 indeed showed a change in behavior from p- to n-type. We further show that by continually replacing the PEt3 ligands by CO ligands, one can control the chemical potential of the semiconductor and even introduce magnetic carriers by controlling the number of ligands, opening a pathway to superatom doped magnetic semiconductors. The talk will highlight the properties of the new semiconductors and how one can use the binding energy of clusters to support as a tool to identify p- or n- type semiconductors.

IL-25: Simple Yet Successful Descriptors for Self-Assembly on Surfaces

Prof. Shobhana Narasimhan
JNCASR, India

Self-assembly is probably the most promising route to constructing devices at the nanoscale. The challenge is to predict the geometries of self-assembled architectures by utilizing only the properties of the individual molecular components. We have explored the feasibility of such an approach for a model set consisting of three host molecules (carboxylic acid derivatives of phenyleneethynylene) and five guest molecules (napthalene, phenanthrene, benzo-c-phenanthrene, benzo-ghi-perylene and coronene), self-assembled on graphene. Using insights gained from scanning tunneling microscopy experiments and density functional theory calculations, we have formulated simple descriptors that can successfully predict the geometries of the host-guest architectures self-assembled from our palette of organic molecules. A structure map can be constructed using host and guest descriptors, with structures of the same type clustering in descriptor space. Though these descriptors can be evaluated atessentially zero computational cost, they correctly reproduce experimental observations, including the structural transitions exhibited by host assemblies upon introducing certain guest molecules. The descriptors are validated by their success in predicting not just the ground state geometry but also the energetic difference between competingstructures for molecules that did not form part of of the training set used when formulating the descriptors.

IL-26: Low-temperature and highly-selective catalysis driven by strong cluster-support interaction between size-selected platinum cluster and silicon substrate

Prof. Hisato Yasumatsu
Tokyo Tech. Japan

It has been found that CO is oxidized on a uni-sized Pt cluster disk bound to a Si substrate, PtN/Si (N=10-60), at as low as 140 K, which is lower by 150 K than on a Pt single-crystal surface. Furthermore, NO is reduced on PtN/Si 70 K lower than on the Pt surface with extremely high selectivity; only N2 but neither N2O nor NO2 is produced even under an excess amount of oxidant, O2. The prominent catalysis of PtN/Si originate from electron accumulation at the sub-nano interface between PtN and the Si substrate as a result of strong electronic metal-support interaction. In the present study, the reaction kinetics and its cluster-size dependence are reported. Bistability was observed in the CO-oxidation kinetics catalyzed by PtN/Si, that is, the reaction rate is different in its heating and cooling processes even at the same partial pressures of CO and O2 as well as the same temperature. This bistability is ruled by balance between more efficient dissociative activation of O2 on PtN/Si and weaker CO adsorption. The wider temperature window of the bistability of Pt30/Si than Pt20/Si indicates the greater ability of the oxygen activation by Pt30/Si owing to an appropriate ratio between the electron-accumulating circumference and the center zone as the reaction field of the Pt cluster disk.

IL-27: Theoretical DFT Study on Modified Oxides and Gold structures

Prof. Nurbosyn U. Zhanpeisov
Tohoku University, Japan

Transition metal oxides and their derivatives are particularly interesting and attractive for wide range of applications because of their technological and industrial importance as catalysts, absorbents, supports, etc. In present talk, we would like to bolster advantages of the cluster approach being relatively simple but complementary to other periodic slab model calculations in proper modeling of extended systems and gold structures as well as in understanding of the molecular level interactions and transformations of the adsorbates on their exposed surfaces. Especially, the structure and chemical activity of the selected transition metal oxide catalysts and gold structures would be thoroughly discussed. Based on these DFT cluster calculations results, some discrepancies with the results of other theoretical investigations and studies in the literature have been critically pointed out.

IL-28: Rational Catalyst Design Augmented with DFT, Machine Learning and Ab-Initio Microkinetic Modeling

Prof. M. Ali Haider
IIT Delhi, India

In search for a sustainable supply of fuels and chemicals, development of green and renewable processes is desirable for mitigating climate change. Towards fulfilling this goal, design of nanoscale materials with desirable level of catalytic or electrocatalytic properties, essentially holds the key to success. In an effort to rationally design catalyst materials, we have adopted a bottom-up approach, wherein quantum mechanical ab initio density functional theory (DFT) simulations of reactions occurring on the material surface are providing a mechanistic rational to design desired catalyst surfaces. The inherent design ideas vary and depend on the problem at hand. Overall, the ab initio level theoretical simulations provide us a mechanistic insight into the reaction, which in-turn offers us an opportunity to engineer the material itself. This is often implemented in experiments by changing the material surface, morphology and the characteristic length scales. Recently we have demonstrated the application of a machine learning (ML) technique in discovering novel catalyst materials for industrial applications. ML based methods are showing potential to significantly reduce the experimental as well as computation cost. Availability of ML algorithms (in open source libraries likeScikit-Learn) and materials database (like CatApp and MaterialsProject) further augments this realization.

IL-29: e-Chemistry of metal oxides – molecule interfaces: data or insights ?

Prof. Kersti Hermansson,
Uppsala University, Sweden

We combine (and develop some) theoretical models & methods including DFT, tight-binding-DFT, and reactive force-fields and machine-learned potentials in a multiscale approach to study metal oxide nano-particles and extended surfaces interacting with molecules and liquids. [1, 2] We have extended the time and length scales above atomistic and simulated O2 temperature programmed desorption (TPD) and H2 temperature programmed reduction (TPR) spectra for ceria nanoparticles. The modelling results neatly explain the positions of the experimental TPD and TPR peaks. [3] This in turn supports a model of oxygen storage on very small metal oxide NPs instead of, or in addition to, inside them. In other ongoing studies we have made long simulations of different water coverages on metal oxide surfaces, using machine learning to generate potentials and fundamental physics models to gain insights. [4-6] The water dynamics and reactivity at metal oxide interfaces are intriguing.

IL-30: Recreating Metal out of Insulators and Insulators out of Metals in Oxide Heterostructures

B. R. K. Nanda
Department of Physics, IIT Madras, Chennai, 600036

Strongly correlated oxides are known to exhibit diverse electronic and magnetic phases due to complex interplay among the charge, spin, orbital and lattice degrees of freedom. Over the last two decades interface engineering has emerged as a new degree of freedom to alter the electronic and magnetic phenomena of these oxides. In this talk, with the aid of the DFT calculations and basic quantum mechanical analysis, we will show that two oxide insulators Sr_2FeMoO_6 and La_2CoMnO_6 create a metallic state when joined together to form a superlattice. We attribute the formation of the metallic state to orbital selective quantization in a periodic potential formed by the superlattice. On the other hand when the metallic Fe_3O_4 forms a superlattice with $NiFe_2O_4$, depending on the period of the superlattice, it replicates the charge order driven metal insulator transition which resemble the Verwey transition.

IL-31: Magnetic Properties of Nd_2CoIrO_6 Double Perovskite

Prof. Subodh Kumar De
IACS, India

The double perovskite Nd2CoIrO6 crystalizes in a monoclinic P21/n structure and is very interesting compound due to containing three magnetic elements Nd3+, Co2+ and Ir4+. Structural analysis as a function of temperature down to 2 K rules out any structural phase transition. Temperature dependent magnetization M(T) under three measurement protocols: zero field cool (ZFC), Field cool cooling (FCC) and field cool heating (FCH) at different magnetic fields reveal ferromagnetic (FM)/ferromagnetic (FiM) transition at about 100 K and antiferromagnetic phase below 25 K. Thermal hysteresis between FCC and FCH M(T) data suggests a spin reorientation phenomenon at low temperature. The shape of magnetization (M) vs. applied magnetic field (H) changes significantly from 2 K to 20 K. Non-saturation of magnetization even up to 5 T indicates a strong coupling between Nd and Co-Ir magnetic sublattices. A sudden change of slope of M-H curve suggests a metamagnetic phase at low temperature. Spin and orbital magnetic moments of Nd3+ and Ir4+ due to strong spin-orbit coupling give rise to rich magnetic phase diagram arising from competitive magnetic interactions along Co-O-Ir, Nd-O-Co and Nd-O-Ir exchange pathways.

IL-32: Exploring the potential of Quadruple perovskites for fast lithium-ion transport

Prof. Hena Das,
Tokyo Institute of Technology, Japan

Suitable solid-state electrolyte materials with high lithium-ion conductivity are indispensable to meet ever increasing demands of solid-state rechargeable lithium-ion batteries to solve various safety and energy density related issues. In this direction, the perovskite family has offered potential candidate materials, Li3xLa(2/3)-xTiO3(LLTO) being the best example, which exhibit high Li+1 conductivity at room temperature. However, these proposed perovskite materials could not be commercialized due to several drawbacks, necessitating expansion of our search in other branches of this family of materials. Therefore, we focus on much less explored members of this family of materials, i.e., Quadruple (AA´3)B4O12 perovskites (where we focus on the d0 transition metal (TM) cations at the B-site), which show several conducive characteristics to model new solid-state electrolyte, such as, (1) A wide variety in structural and chemical compositions, (2) Presence of transition metal cations with multiple potential oxidation states at the A-site and (3) Tendency to form layered A-site cation ordered structure that could facilitate lithium-ion diffusion. We will first discuss the properties of the synthesized candidate Li4/3Cu4/3Ta4O12, which is found to stabilize in a Li-Cu-□ ordered structure which forms 1D lithium-ion diffusion pathways. We will also discuss how the characteristics of this category of materials lead us to formulate guidelines to design materials with improved functionalities. We first screened candidate materials on the basis of their chemical composition, band gap and estimated lithium-ion conduction energy barrier height. In course of this presentation, we shall also deliberate upon our investigations on the thermodynamic and chemical stability of the selected binary and ternary candidates based on the cluster expanded lattice model Hamiltonian and finite temperature Monte Carlo simulations as we had successfully applied to study configurational order in the lithium nickel complex oxide battery materials [Hena Das et. al., Chem. Mater. 29, 7840−7851 (2017)].

IL-33: An Interesting Application of Desiccation Crack Networks in Technology

Prof. Sujata Tarafdar
Department of Physics, Jadavpur University, Kolkata 700032, India

Fracture is a very important area of study in engineering, geology, material science and several other fields, but usually for its negative impact. Recently the network of cracks formed in layers of drying colloidal suspensions, have been used in an innovative way to produce transparent conducting surfaces which find applications in a wide variety of devices. The ‘crackle method’ to be discussed here, has been developed by the Bengaluru group led by Prof. G.U. Kulkarni and provides a simpler and more cost effective alternative to ITO coated glass or its substitutes normally used for such purposes. We also discuss some simple simulation studies of desiccating films, attempting to identify how to create the crack network most effective for the purpose.

IL-34: Controlled crack patterns produced by memory effect of paste

Prof. Akio Nakahara
College of Science and Technology, Nihon University, Japan

A densely packed colloidal suspension, called a paste, remembers the direction of applied forces and, when it is dried and desiccation cracks are formed, the direction in which the dried paste is easy to be broken is determined by the memory of applied forces (memory effect of paste). For example, when a paste remembers the direction of vibrational motion, all primary desiccation cracks propagate in the direction perpendicular to the direction of the vibrational motion that the paste has experienced. On the other hand, when a paste remembers the direction of its flow motion or the applied magnetic field, all primary cracks propagate along the direction of its flow motion or the applied magnetic field. The paste can remember the direction of these applied forces due to its plasticity, but the ways that the paste remembers the direction of each applied force are different from each other. The memory effect of vibration can be explained by the residual tension theory which states that the residual tension is produced horizontally under oscillatory shear motion. As for the memory effect of flow or magnetic field, the chain formation of colloidal particles along its flow motion or the applied magnetic field is considered to play a dominant role in memory effect. The memory of paste can be rewritten by additional applied force and can be erased by irradiation of ultrasonic waves to the paste. As the application of memory effect of paste, we can control the morphology of crack patterns by imprinting, rewriting and erasing memories in paste and produce various types of crack patterns, such as striped, radial, ring, spiral, lattice and random structures.

IL-35: Computational materials design from materials simulations to informatics

Prof. Kenta Hongo,
JAIST, Japan

Materials Informatics (MI) [1] has attracted enormous attention in materials science. About a decade ago, computational material design relied only on materials simulations, considering a small search space limited to tens to hundreds of compounds. On the other hand, MI such as high-throughput virtual screening approaches based on machine learning techniques expands its search space into that in the order of hundred thousands of compounds. In particular, ab initio simulations based on density functional theory (DFT) have been widely used to generate various materials property data. Although DFT succeeds in describing most property predictions, but it fails in some cases (e.g., strongly correlated systems, noncovalent systems, etc). One of the most practical approaches to circumventing the DFT failures is quantum Monte Carlo (QMC), especially diffusion Monte Carlo (DMC). QMC stochastically solves the many-body Schrödinger equation with a good balance between accuracy and computational cost, and hence is quite suitable for recent massively parallel computers because of its high parallel efficiency. For the next-generation exascale supercomputers, QMC can be used as one of the next generation "data generation engines" in the "ab initio MI". In this talk, I will present a brief introduction to MI followed by our recent achievement [2] as well as materials simulations [3,4].

IL-36: Theoretical design and development of new macrocycle organic materials for organic electronic applications

Dr. Mahesh Kumar Ravva
SRM University – AP, Andhra Pradesh 522503

In this work, several conjugated donor-acceptor macrocyclic molecules were designed using density functional theory methods. These molecules can be used as electron donor and electron acceptor materials in organic solar cells. The structural and electronic properties of these molecules were evaluated and compared with the linear molecules. Further, we have studied the nature of the interaction between these new macrocyclic acceptors and common donor polymers. It is found that the macrocyclic acceptor has shown better electronic properties and enable 3D charge transport properties. The results obtained from this investigation could aid in the development of organic solar cells with higher power conversion efficiency.

IL-37: Quasiparticle energies of ground state and excited state of metal clusters using all-electron mixed basis of plane waves (PWs) and atomic orbitals (AOs)

Prof. Vannajan Sanghiran Lee
University of Malaya, Malaysia

Quasiparticle energies of optimized geometry of metal clusters in Group I were explored and evaluated from ab initio calculation by GW approximation. All-electron mixed-basis approach by a linear combination of both plane waves (PWs) and atomic orbitals (AOs), was applied in order to deal with the core electrons accurately with TOMBO code. The code doesn’t use the pseudopotentials but adopt the all-electron mixed-basis orbitals. The GW approximation for the photoemission (quasiparticle) spectra, the Bethe–Salpeter equation (BSE) approach for the photoabsorption spectra, and T-matrix approach for the Auger (two particle) spectra can be the accurate methods for the excited states. By using the GW approximation, absolute energies will be determined, and, finally not only the ionization potential, electron affinity and energy gap, but also all excitation spectra in a single calculation will be obtained accurately. Contributions to the quasiparticle energies in eV for the HOMO and LUMO levels were explored and compared. Excited state calculation for photoabsorption energy spectra for the clusters were also investigated and discussed.

IL-38: Computational Evaluation of Donor-Bridge-Acceptor (D-B-A) Motifs for High Performance Optoelectronic Device Applications

Prof. V. Subramanian
CLRI, India

Donor-Bridge-Acceptor (D-B-A) systems are used in a variety of devices, including phosphorescent organic light emitting diodes (PhOLEDs), organic field-effect transistors (OFET), dye sensitized solar cells (DSSC), polymer solar cells (PSCs) and Thermally Activated Delayed Fluorescence (TADF). Hence, exploring electronic structure calculation of D-B-A systems is an important research field which yields necessary information to develop materials for future optoelectronic applications. It is important to understand how to control and modulate the frontier molecular orbitals (FMO), i.e. highest occupied molecular orbital (HOMO) and lowest unoccupied molecular orbital (LUMO) with respect to the neighboring layers in the device. The aim of present talk focus on the following topics, related to PhOLEDs, DSSC and TADF applications: 1) Discussion on the rational design rules for bipolar host materials for the blue PhOLEDs. 2) Theoretical design of core modified (oxa and thia) porphyrin based organic dyes for DSSC applications. 3) Electronic structure of the triazine based organic molecules for TADF applications.

IL-39: Mechanics and Mechanisms of Deformation and Failure in Heterogeneous Amorphous Alloys: Insights from Continuum Simulations of Porous BMGs and ex-situ BMG Composites

Prof. Parag Tandaiya
Department of Mechanical Engineering, Indian Institute of Technology Bombay, Mumbai

Single phase amorphous alloys or monolithic bulk metallic glasses (BMGs) lack macroscopic ductility as they are susceptible to catastrophic failure along a dominant shear band soon after yielding begins in uniaxial loading at room temperature. To overcome this drawback of monolithic BMGs, heterogeneous amorphous alloys such as porous BMGs and secondary crystalline phase reinforced ex-situ BMG matrix composites have been synthesized by researchers. Experiments suggest that porous BMGs can exhibit large malleability in uniaxial compression with very little loss in strength. Similarly, ex-situ BMG matrix composites show improved performance in experiments. However, a thorough understanding of the underlying deformation mechanics and mechanisms is lacking in literature. In this presentation, the mechanics and mechanisms of deformation and failure of both low porosity BMGs and high porosity BMG foams under uniaxial compression will be elucidated by gaining insights from three-dimensional finite element simulations. The effect of various stress states on the deformation and failure of a porous BMG will also be examined. The deformation and failure mechanics of ductile particle, short fiber and long fiber reinforced ex-situ BMG composites will also be discussed. Finally, the mechanistic origins of work hardening observed in recently developed Shape Memory Alloy particle reinforced BMG matrix composites will also be elucidated.

IL-40: Kolmogorov Dispersion for Turbulence and Statistics of Fracture in the Fiber Bundle Model

Prof. Bikas K. Chakrabarti
SINP, India

It has long been conjectured that (rapid) fracture propagation dynamics in materials and turbulent motion of fluids are two manifestations of the same physical process. The universality class of the Turbulence (Kolmogorov dispersion in particular) had been conjectured to be identifiable with the Flory statistics for linear polymers (self-avoiding walks on lattices). The statistics of fracture in the Fiber Bundle Model are now well studied and many exact results are now available for the equal load-sharing (ELS) scheme. Seems, the correlation length exponent in this model was missing and we show here how the correspondence between fracture statistics and the Flory mapping of Kolmogorov statistics for turbulence helps us obtaining the exact value of the correlation length exponent for fracture in the ELS limit of FBM., and also the upper critical dimension.

IL-41: Electronic Descriptor for carbon catalyst using QM/ML approach

Prof. Ranjit Thapa
Department of Physics, SRM University – AP, India

Oxygen evolution reaction (OER) is a key aspect of energy conversion and storage technologies. The optimal electro-catalyst can speed up the sluggish kinetics of OER. It is important to understand the potential determining step which defines the activity**.** Recently, descriptor based approach becomes efficient to search and design the correct catalyst for various reactions. Also for OER carbon based materials come up with ideal electronic properties and advantages in CO tolerance, surface area, cost, abundant etc. To find the identical carbon catalyst in large material space is a big task for the research community in this area. We address these challenges using density functional theory to understand the role of O intermediate to define the activity and how Machine learning assisted DFT calculation can help to design catalysts for OER. The π electron plays a role in the adsorption of intermediates that defines the activity of carbon site in graphene nanoribbons (GNRs). We developed predictive models using machine learning algorithms to estimate the site-specific catalytic activity of GNRs. These predictive models can help in the quantitative estimation of the atomic site-specific OER activity for carbon based electrode catalyst by reducing the computational effort.

IL-42: Ab initio Quantum Monte Carlo method; Role in Materials Genome

Prof. Ryo Maezono
JAIST, Japan

The ab intio Quantum Monte Carlo method is another universal framework to achieve electronic structure calculations to be compared with other approaches like DFT (density functional theory) or MO (molecular orbital methods). It solves the ab initio Schrodinger equation without taking one-body forms, by using numerical Monte Carlo samplings applied directly to many-body wave functions, not decomposed into orbital functions [1]. Because of less assumptions required, the method achieves more reliable ab initio evaluations especially on the electronic correlations over DFT or MO. With high parallel efficiency achieving around 99%, the method is rapidly getting more practical to be used over such problems like magnetism [2-4], surfaces[5,6], inter-molecular interactions [7-11], and other fundamental problems[12-14], those forming generally difficult challenges to the conventional DFT and MO. Unlike DFT with the ambiguities due to the choice of exchange-correlation functionals, or MO with the complexities in the various correction schemes indispensable, the QMC realizes simpler and straightforward evaluations toward high accuracy. These advantages push the ab initio QMC method to be a promising 'killer application' running on flagship supercomputers in US for Materials Genome, with the highest efficiency to extract the power of massive parallel computations. In the talk, we present our group's efforts for decades using several implementations like CASINO[4,7-14], QMCPack[6], and TurboRVB[15].

IL-43: Analysis of heat flow visualization and thermodynamic efficiency during thermal convection in cavities with distributed solar heaters

Prof. Tanmay Basak,
IIT Madras, India

The phenomenon of natural convection plays a significant role in various industrial and thermal processing applications. The conventional method of differential heating within an enclosure may result in the inadequate thermal mixing and that may further lead to the poor thermal management. In order to enhance the overall thermal mixing, the discrete heating strategy may be considered as an attractive alternative. The major application of discrete heaters along the side walls is solar thermal induced natural convection. The single or double discrete heaters are positioned at various strategic locations along the side walls of the triangular (type 1 and type 2) and square cavities in order to enhance the effective mixing of fluid in the entire enclosure. This lecture elucidates natural convection within discretely heated square and triangular (type 1 and type 2) enclosures filled with fluid and porous medium. Overall, five test cases based on the single heater arrangement (cases 1a-1e) and three test cases based on the double heater location (cases 2a-2c) along each side wall have been considered for the present work. The heatline method has been implemented to visualize the heat flow pattern within the cavities for a wide range of parameters involving various dimensionless numbers. In order to solve the governing equations and Poisson equations for streamfunction and heatfunction, the Galerkin finite element method has been used. Heatlines are effective in explaining the complex heat flow patterns from the various discrete heating sources in the cavities. Further, the local and average Nusselt number are largely effective in illustrating the heat transfer distribution along the isothermal walls and discrete heaters. Lastly, the extent of thermal mixing is quantitatively measured using the cup-mixing temperature whereas the uniformity in the temperature distribution is evaluated using the root mean square distribution in each distributed heating case (cases 1a-1e and cases 2a-2c). The energy efficiency of the various distributed heating strategies has been carried out using the irreversibility or entropy generation estimates. The entropy generation minimization approach has been implemented in order to analyze the destruction of available energy for the various thermal processing applications. The local maps of heat transfer and fluid friction irreversibilities are obtained for the various distributed heating strategies. Also, the heat transfer and fluid friction dominance during conduction or convection dominant regime has been studied. In order to accurately estimate the entropy generation terms, a finite element based numerical procedure has been developed. The current algorithm has been validated with that of the previous works and they are found to be in excellent agreement. The heatline investigation involving fluid media case clearly illustrates the conduction dominance at low Rayleigh number based on the end to end parallel heatlines whereas convective heatline cells are observed along with the wall to wall heatlines at high Rayleigh numbers. Common to all the cases, the heatline analysis involving porous media exhibits the onset of convection at lower Darcy number whereas enhanced convection is found to occur at high Darcy number based on the presence of intense fluid and heatline cells irrespective of Prandtl number. At the low Rayleigh and Darcy numbers, the dominance of entropy generation due to heat transfer is found to be higher over fluid friction whereas at the higher Rayleigh and Darcy numbers, the entropy generation due to fluid friction is largely dominant over thermal irreversibility within the cavities. Overall, the heatline and entropy generation analysis clearly demonstrates that distributed/discrete heating results in the enhanced thermal mixing and a larger extent of temperature uniformity throughout a large region in the square and triangular (type 1 and type 2) cavities for all types of fluids. Based on the thermal mixing studies, it may be inferred that the triangular-type 2 and square configurations exhibit significant thermal mixing compared to the triangular-type 1 cavity. On the other hand, triangular-type 1 cavity demonstrates greater rate of heat transfer compared to square and triangular-type 2 cavities. This lecture also concludes that the effective utilization of energy resources for the processing of materials may be achieved by the thermal management policy based on the distributed heating strategy which significantly enhances the thermal mixing and temperature distribution in the square and triangular (type 1 and type 2) cavities with higher energy efficiency.

IL-44: Controlling plasmonic characteristics through confinement and correlation effects

Prof. MAJIDI Muhammad Aziz
University of Indonesia

Recent discoveries of plasmons with new characteristics, introducing the term unconventional plasmons, have enriched the field of plasmonics and condensed-matter physics in general. Unconventional plasmons refer to collective excitation of bound electrons, which can occur in materials being in non-metallic phase. These plasmons can emerge in strongly-correlated materials due to Coulomb correlation effects, or in weakly-correlated materials due to confinement or size reduction of the system, such as in nanoparticles, or both effects may contribute in some systems. Motivated by our current experimental study on optical responses of gold nanoparticles, whereby the samples behave in many respects like insulator, here we attempt to provide a theoretical explanation for such a system. We construct a finite-size tight-binding-based Hamiltonian incorporating s-d hybridization and on-site Coulomb repulsion on the d orbital. Our results qualitatively agree with the experimental data and suggest that noble metals such as gold behave as regular metal showing conventional plasmonic behavior when in bulk, but become correlated insulator exhibiting unconventional plasmonic behavior in nanoscale size. The unconventional plasmonic energy may be controlled by tuning the nanoparticle size or by the choice of material with suitable hybridization and on-site Coulomb interaction strength.

IL-45: Catalysis on the surface of nanotubes having confined solvent media

Prof. Kothandaraman Ramanujam
IIT Madras, India

In the literature, many kinds of reactions have been described to take place within the carbon nanotubes (CNTs) due to nanoconfinement. We have shown the confined species to exhibit an electronic communication through the walls of CNTs to the species interacting with CNTs on its outside surface. The liquid-filled multi-walled carbon nanotubes (MWCNTs) exhibit remarkably enhanced characteristics for sensor applications, the detection threshold being lowered by as much as an order of magnitude, while detection sensitivity is doubled for a number of molecules including ascorbic acid, dopamine, and uric acid [1]. 1H NMR relaxometry at a moderately low field, i.e 14.6 MHz (0.34 T), confirms that the improved sensor characteristics are correlated with the filling of MWCNTs with solvents such as acetonitrile, dimethyl sulfoxide, etc. The molecular motions are slowed down when solvent molecules fill MWCNTs, thus increasing motional correlation times and hence longitudinal relaxation rate increases under extreme narrowing conditions. The filling of MWCNTs appears to relate to solvent-CNT interactions that are in line with the principle of hard and soft acids and bases, and also correlates with solvent dipole moments. We have further enhanced the detection limit and selectivity towards ascorbic acid by modifying the solvent confined MWCNTs surface with 1-amino 2-napthol. Effect of endohedral filling is also capitalized in enhancing the redox chemistry of the battery. A high voltage redox couple (~0.9 V vs. SHE), dopamine/dopamine quinone (and its derivatives) was used along with V2+/V3+ redox couple (-0.25 V vs. SHE) to realize a ~1.2 V flow battery. Dopamine/dopamine quinone shows highly reversible behavior in 3 M H2SO4 while using acetonitrile confined MWCNTs coated graphite felt as electrode.

IL-46: Theoretical and Mechanistic Studies on Catalysis of Carbon Dioxide Hydrogenation to Formic Acid on Pt doped Boron Nitride Nanosheets

Prof. JUNGSUTTIWONG Siriporn
URU, Thailand

The catalytic conversion of carbon dioxide to valuable compounds such as formic acid, formaldehyde, and methanol has received much attention from the industrial and environmental sectors. We investigated the reaction mechanism for CO2 hydrogenation to formic acid on Pt-doped boron nitride nanosheets (Pt-BNNS) and Pt boron-vacancy (Pt-BV) by using density functional theory (DFT). There are two possible reaction mechanisms, namely, H2 dissociation and co-adsorption. We found that co-adsorption with the second dissociation of hydrogen molecule are the more favorable mechanism on Pt-BV, and produces formic acid via a carboxylate intermediate (COOH). The reaction is exothermic, with activation energy for the rate-determining step, of 0.78 eV. The CO2 hydrogenation via the co-adsorption mechanism is a thermodynamically favorable process on Pt-BV, with a negative Gibbs free energy value. The presence of H2 molecule in system may play a role in producing the formic acid. Our calculation results provide a justification for development Pt-BV-based catalysts for the hydrogenation of CO2 and the conversion of greenhouse gases to value added products.

IL-47: Lubrication Driven Hierarchical Self-Assembly of Droplets

Prof. V. Madhurima,
Central Uni. Tamil Nadu, India

Hierarchical structures enhance wetting properties. Vapours of liquid drops self-assemble into hexagonal structures over any cold surface and the presence of a lubricating layer between the substrate and a slowly drying polymeric layer leads to hierarchical patterns of these condensation droplets. The formation of these hierarchical structures is not well understood. Attempts have been made to explain them using either cracks due to surface stresses or as due to depinning of the three-phase contact line formed by the condensing droplets. In this talk, I will first discuss the general ideas of self-assembly of droplets, the role of fluid instabilities and the coffee stain effect. The influence of an intermediate lubricating colloidal layer (milk) of varying concentrations on the pattern of the self-assembled droplets will be examined from their confocal microscope images. It will be seen that the presence of a lubricating layer enhances wetting properties – both hydrophilic and hydrophobic.

IL-48: Yielding at bulk and Nanoscale amorphous solids

Prof. Smarajit Karmakar
TIFR Hyderabad, India

Understanding the failure mechanisms of amorphous solids under external load is one of the most active research fields in materials physics and engineering. It is experimentally known that amorphous solids have often a much larger failure strength than their crystalline counterparts with similar compositions, but they may also show catastrophic failure which severely limits their applicability as useful design materials. Bulk materials that exhibit catastrophic failure by forming cracks under an applied load are generically termed as brittle materials, as opposed to ductile materials that show significant plastic deformation before final failure. Using numerical simulations, we have studied the yielding response, in the athermal quasi-static limit, of a model amorphous material having inclusions in the form of randomly pinned particles. We show that, with increasing pinning concentration, the plastic activity becomes more spatially localized, resulting in smaller stress drops, and a corresponding increase in the magnitude of strain where yielding occurs. We demonstrate that unlike the spatially heterogeneous and avalanche led yielding in the case of the unpinned glass, for the case of large pinning concentration, yielding takes place via a spatially homogeneous proliferation of localized events. If time permits I will also discuss our recent work on yielding of amorphous solids at the nanoscale. Amorphous solids, confined on the nano-scale, show failure patterns different from the bulk system. Such systems are strongly affected by the confinement geometry and interfacial effects. We studied a confined model glass, subjected to uniaxial loading, for varying aspect ratio of the sample geometry. While for small aspect ratio, the sample breaks by forming a neck, above a critical value of the aspect ratio, cavitation is seen. The critical aspect ratio is associated with a strain-rate and temperature-dependent critical curvature of the neck, above which the free energy of the system is minimized by the formation of a cavity. We believe that this mechanism of cavity formation is probably a generic mechanism for material’s failure in small confined systems under mechanical load.

IL-49: Stick-slip in soft polymers: Elasticity, adhesion and slow wave propagation

Prof. Koushik Vishwanathan
IISc Bangalore, India

Stick-slip is a friction instability that governs diverse phenomena from squealing automobile brakes to earthquakes. The origin of this instability has conventionally been explained using rigid slider models with a rate-and-state type friction law. Recent high-speed experimental imaging of adhesive polymer contacts has shown that stick-slip is intimately governed by both the elastic dynamics of the sliding body and interfacial adhesion. Furthermore, the resulting intermittent motion is mediated primarily by the propagation of interface slip waves of elastic origin---three fundamentally distinct waves exist and correspond to three different modes of stick-slip with their own characteristic features. This talk will review some of these experimental results and describe a theoretical framework to explain the occurrence of these waves. The micromechanisms underlying these waves, their physical origin and consequences on the macroscale will be discussed.

Young Researcher Presentations

YRP-1: Searching of suitable cationic dopants for CZTS/Se using First-Principles study

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Abstract:

The art of designing futuristic materials with low-cost and eco-friendly benign component elements for the generation of new photovoltaic thin film solar cells with high efficiency remains a challenging issue. As an earth-abundant, high absorption coefficient (10^4 cm^{-1})[1], desire optical direct band gap (1.0-1.5 eV)[2], Kesterite $Cu_2ZnSn(S/Se)_4$ (CZTS/Se) is considered to be a next generation absorber material for solar cells. The present conversion efficiency of CZTS/Se-based solar cells (9.4 /11.6 %)[3] can be further be improved by adding of dopants to the absorber layer. In this regard, we have performed First-principle calculations for Sb, Al, Ga, Ba-doped CZTS/Se structures using HSE06 hybrid functional. The stable chemical potential region is obtained through the examination of thermodynamic stability of the compound by avoiding the formation of secondary phases such as Cus/Se, Cu_2S/Se, ZnS/Se, SnS/Se, $Sn(S/Se)_2$ and $Cu_2Sn(S/Se)_3$. This will control the elemental chemical potential during crystal growth. Zn-rich and Cu, Sn-poor conditions are required to prevent their formation and increase the efficiency. We calculated the formation energies for checking the existence of intrinsic point defect in the material and it is directly depend on the chemical potentials of the related elements. Furtherly we examine the current density and upper limit of the energy conversion efficiency P (%) of CZTS/Se materials. Our results demonstrate that the lower formation energy, preferable energy gap and excellent optical absorption of the Sb doped CZTS/Se make it potential component for relatively high efficient solar cells.

Keywords: Kesterite; Doping; Formation Energy; DFT; current density; power conversion efficiency P (%)

References:

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YRP-2: Exploring the Efficiency of Carbon Nanostructures for Hydrogen Storage and Oxygen Reduction Reaction

Dr. Paramita Banerjee
JNCASR, India

First-principles density functional theory has been employed to explore new carbon allotropes such as, carbon nanohorn and T6-carbon for the purpose of hydrogen storage and oxygen reduction reaction (ORR) respectively. In this presentation, I will explain how the presence of curvature can be exploited as a tuning parameter to activate the hydrogen storage capability of single-walled carbon nanohorns (SWCNHs). The binding strength of ad-atoms on SWCNHs of different curvature is correlated with the π electron occupancy of the corresponding carbon ring. Higher π electron occupancy causes significantly high binding energy of the metal ad-atoms (M), thereby indicating high stability of those M-C bonds. After full hydrogenation, Li-doped SWCNHs are found to contain a maximum of 7.5 wt. % of hydrogen. Overall, our results indicate that Li-doped SWCNHs with intra-curvature values higher than 11^{o}, is a potential candidate for hydrogen storage. I will also explain the electro-catalytic activity of a new carbon allotrope i.e. T6[100] surface containing both sp3 (C1) and sp2 (C2) hybridized carbon atoms for efficient ORR. As estimated from free energy profile, the overpotential is much lower when C1 is considered as the active site and the final step i.e. desorption of final OH- ion is found to be the potential determining step. Thus, the presence of both sp2 (maintains the high metallicity needed to reduce ohmic loss) and sp3 (helps in capturing the upcoming molecules) hybridized carbon atoms in T6[100] surface helps it to act as a potential candidate for ORR.

YRP-3: Brittle to quasi-brittle transition in a compound fiber bundle

Dr. Chandreyee Roy
Satyendra Nath Bose National Centre for Basic Sciences, Kolkata-700106, India

The brittle to quasi-brittle transition has been studied for a compound of two different kinds of fibrous materials, having distinct difference in their breaking strengths under the framework of the fiber bundle model. A random fiber bundle model has been devised with a bimodal distribution of the breaking strengths of the individual fibers. The bimodal distribution is assumed to be consisting of two symmetrically placed rectangular probability distributions of strengths p and $1 - p$, each of width d, and separated by a gap $2s$. Different properties of the transition have been studied varying these three parameters and using the well known equal load sharing dynamics. Our study exhibits a brittle to quasi-brittle transition at the critical width $dc(s, p) = p(1/2 - s)/(1 + p)$ confirmed by our numerical results.

YRP-4: Effective rheology of two-phase flow in porous media: dependence on system disorder

Dr. Subhadeep Roy
Norwegian University of Science and Technology (NTNU), NO-7491 Trondheim, Norway

When two immiscible fluids flow in a porous media the flow does not obey linear Darcy law in the regime where the capillary forces are comparable to the viscous forces. The flow rate was observed experimentally to scale in a quadratic manner with the pressure gradient for two-dimensional Hele-Shaw cells as well as a three- dimensional porous medium constructed with glass bids. The disorder in capillary barriers at pores effectively creates a yield threshold, making the fluids reminiscent of a Bingham viscoplastic fluid in the porous medium, introducing an overall threshold pressure Pt in the system. Due to disorder in capillary barriers, an increasing number of connecting paths appear in the system while increasing the pressure gradient (ΔP), enhancing the increase of overall flow rate Q more faster than the linear dependence. This leads to a quadratic dependence of Q on the excess pressure drop (ΔP-Pt) at the capillary dominated the regime and a linear dependence at a sufficiently high flow rate when all pores open up. The disorder in the capillary barriers at the pore the level appears due to two factors: (i) fluctuation in pore sizes and (ii) interface configurations between the two fluids inside a pore. At very high ΔP, when the fluid flows through all possible connecting paths, Q increases linearly with (ΔP-Pt). We have adopted a 1d prototype of porous media called the capillary fiber bundle model [6] and explored this transition from non-linear to linear behavior with increasing flow rate or pressure gradient and relate this dynamics with increasing number of active paths as the model evolves with time. We observe a strong connection between the dynamics of active paths with the effective rheology of the system. The system is then explored numerically in two dimensions as well with varying pressure gradient while the viscosity ratio and surface tension is kept fixed. The findings in both 1d and 2d are in good agreement to the experimental observation.

YRP-5: Elucidating the origin of capacity fading of Ni-rich layered oxide-based positive electrode materials for Li-ion batteries

Dr. Mudit Dixit
Lovely Professional University, Phagwara, Punjab, India

Lithium-rich layered transition metal oxides of nickel, cobalt, and manganese (NCMs) are one of the most promising positive electrode materials of lithium ion batteries which meet the requirements of energy density in electric vehicles and hybrid electric vehicles. Although these materials are attractive, the capacity of these materials fades rapidly on cycling, the factors that govern the stability of these materials remain unclear. In absence of the knowledge of these factors, the promise of commercialization of Li-rich positive electrode materials for Li-ion batteries is likely to remain difficult. In this work, we performed a systematic study of NCMs with varying metal composition using first principles based computational methods towards the identification of the factors that govern the stability and electrochemical properties of these materials. The obtained results can guide experiments to accelerate the discovery of stable and effective electrode materials.

YRP-6: Excitation energies from thermally-assisted-occupation density functional theory: Theory and computational implementation

Dr. Aaditya Manjanath
Institute of Chemistry, Academia Sinica, Taipei City, 115, Taiwan

The linear response (LR) time-dependent density functional theory (TDDFT) has been broadly used to investigate excited-state properties of various molecular systems1,2. Although, extremely useful for a plethora of finite systems, the results from this method can be inaccurate for systems with small highest-occupied/lowest-unoccupied molecular orbital (HOMO-LUMO) gaps due to non-dynamical (static) correlation. Traditional treatment for such systems involves active-space formalisms that can scale factorially with size. An attempt was made recently by Chai to circumvent this challenge, in the form of a thermally-assisted-occupation (TAO) DFT scheme. This method explicitly incorporates the non-dynamical correlation effect in the ground-state simulation, but retains the low computational complexity of conventional DFT. The aim of this work is to combine ground-state TAO-DFT with the LR-TDDFT framework to study excited-state phenomena. The preliminary simulations successfully capture the dissociation feature of the first triplet excited state of the hydrogen molecule, which is not the case for both, conventional TDDFT as well as TDHF methods.

YRP-7: Understanding the chemical enhancement mechanism of 2D substrate enhanced Raman Spectroscopy (2D-SERS).

Dr. Kanchan Ulman
Department of Physics, National University of Singapore, Singapore.

Surface-enhanced Raman spectroscopy (SERS) is a well established field which utilizes the enhancement of Raman signals for molecules on metal substrates, resulting in applications of this phenomena for detection and identification of trace concentrations of molecules. In recent years, two-dimensional (2D) materials like graphene, h-BN and MoS_2 are being used as substrates for SERS, giving rise to rapidly growing field of 2D-substrate enhanced Raman spectroscopy (2D-SERS). In conventional SERS, the enhancement factor is dominated by an electromagnetic enhancement mechanism, as compared to the smaller chemical enhancement effect. In 2D-SERS however, this chemical enhancement effect (which stems from electron-phonon coupling within the molecule and substrate) is thought to play a dominating role. Yet, the detailed understanding of the chemical enhancement effect in 2D-SERS is still lacking. Using first principles calculations, we study the chemical enhancement mechanism using typical probe molecules such as pyridine and pthalocyanine on 2D substrates, highlighting the role of electron-phonon coupling and charge-transfer excitons in the chemical enhancement mechanism of 2D-SERS.

YRP-8: Predicting the collapse point of materials under stress

Prof. Srutarshi Pradhan
NTNU, Norway

Fiber bundle model (FBM) captures correctly the stress-induced failure behavior of disordered materials under external loading. In general, the non-linear stress strain curve (load curve) assumes a parabolic shape and the maximum point of the load curve gives the strength of the system. The system goes unstable after crossing that maximum point (failure point) and catastrophic failure occurs (the system collapses). We have calculated the elastic energy and damage energy of an equal-load-sharing FBM during the entire failure process. While the damage energy gradually increases with strain, the elastic energy shows a peak in the unstable phase of the system. In addition, the slope of the elastic energy versus strain curve has a maximum that appears always before the failure point (in the stable phase of the system) --- therefore it can be used as a reliable signal of upcoming catastrophic failure. The theoretical analyses are done for power law type and Weibull distributions of fiber thresholds and all the theoretical estimates are verified by numerical simulations on a single FBM having large number of fibers (10 Million).

Oral Presentation

O-1: High-throughput Screening of Single Transition Metal Atoms Anchored on MoS_2 Monolayer for Nitrogen Fixation

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Abstract:

The electrochemical nitrogen reduction reaction (NRR) at ambient conditions is emerging as a promising alternative pathway to the energy-intensive and centralized Haber-Bosch process for ammonia synthesis. In addition to nitrogen-doped carbon or boron nitride, coordinated Sulphur atoms have been also proposed to anchor single atom catalysts (SACs) and tune their catalytic performance. Herein, by means of high-throughput first-principles calculations, we choose molybdenum disulfide (MoS_2) monolayer as a model substrate material and explore the feasibility of a collection of sulfur-stabilized single transition metal atoms towards NRR. We find that the single molybdenum atom anchored on MoS_2 has the best NRR performance with an estimated overpotential of around 0.3 eV via the distal mechanism. Our calculations also confirm the selectivity to NRR against hydrogen evolution reaction (HER) as well as the stability of the Mo SAC anchored on MoS_2.

Keywords: Electrocatalysis; High-throughput calculations; Nitrogen reduction reaction; Molybdenum disulfide; Single atom catalysts

O-2: Combining DFT with ML to study size specific interactions between metal clusters and adsorbates.

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Abstract:

To date, density functional theory (DFT) is one of the most accurate and yet practical theory to gain insight about materials properties. Although successful, the computational cost is the main hurdle even today. A way out is combining DFT with machine learning (ML) to reduce the computational cost without compromising accuracy. However, the success of this approach hinges on the correctness of the descriptors. In the present work, we demonstrate that, based on *only* interatomic distances as descriptors, our ML model predicts interaction energy between an adsorbate and Al cluster with mean absolute error (MAE) ~ 0.05 eV (or less) and reproduces the PES experienced by an incoming atom. Our extensive DFT calculations reveal that atoms experiencing identical environment within a cluster have identical interaction energy patterns. Further, we demonstrate that our model is not specific to Al clusters, and could be applied to clusters of different elements as well. Its application to compute PES experienced by various test atoms and molecules in the vicinity of different clusters proves the transferability of the model not just to clusters of different elements but also to various molecules. The descriptors chosen are invariant to rotation, translation, and permutation yet very simple to compute is one of the most crucial points of the present work.

Keywords: clusters; reactivity; DFT; ML

O-3: Rational Design of Single Atom Catalysts based on Cu, Ag and Au alloys using Machine Learning Approaches

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Abstract:

In heterogeneous catalysis, computational modelling has significantly improved the understanding of surface chemistry. Density functional theory (DFT) is the most commonly used computational method which gives the insight into reaction mechanisms which supports catalyst development that can be later verified experimentally. Till now, DFT calculations are using binding energy as a descriptor in search of a more catalytically active catalyst. In addition, it is also undeniable that computational time and cost in DFT is very high. Therefore, Machine Learning (ML) algorithms (through open source libraries like Scikit-Learn) are being utilized and different ML based models are developed. An extensive study has also been reported to provide a better understanding of different ML models and also find the most promising model among them. In addition, availability of materials database (like CatApp, Materials Project) is also taken into account while developing these algorithms, which eventually predicts the oxygen and carbon binding energy of single atomic alloys (SAA). Further, readily available periodic table properties of metals are utilized as features in the model and it has been found that gradient boosting regression (GBR) predicted binding energies are more promising as compared to other ML algorithms (like Linear Regression, Support Vector Regressor, Random Forest Regressor, and Extra Tree Regressor)[1]. The computational time in GBR was found to be 0.0006 s on a dual-core computer which is very less as compared to DFT calculations. Therefore, ML techniques are showing promising future in the field of heterogeneous catalysis which can enhance the process of catalyst development.

Keywords: catalyst; machine learning (ML); binding energy; density functional theory (DFT)

References

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O-4: Thermal analysis of Myristic - Layric acid –Fe_2O_3 composite as nano-enhanced organic phase change material

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Abstract:

Phase change materials (PCM) are commonly utilized materials in latent heat energy storage (LHES) systems. In the present study, Fe_2O_3 was incorporated into lauric acid and the eutectic mixture of myristic acid and lauric acid respectively. The composites were prepared by melting and mixing method. To observe the surface morphologies of Fe_2O_3 and nanocomposites atomic force microscopy. The images from AFM confirmed the homogeneous distribution of Fe_2O_3 in the composite. Fourier transform infrared spectrum (FRIR) results revealed that the eutectic mixture is having chemical stability. The acids dispersed with iron oxide were prepared to enhance the thermal properties of the PCM mixtures and heat transfer at various Fe_2O_3 loadings of 1 wt. %, 2 wt. %, 3 wt. %, 4 wt. % and 5 wt. %, were investigated. It was observed from the experimental results that the duration of melting and cooling rates for PCM composites increased in all nano compositions with respect to the their pristine counterparts.

Keywords: Phase change material; Lauric acid - Myristic acid; Eutectic mixture; Fe_2O_3; Heat transfer.

O-5: First Principles Study of Structural, Electronic, Magnetic and Elastic Properties of the Mn_2-X-Sb (X= Co, Fe) Inverse Heusler Alloys

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Abstract:

We predicted the ground state properties, electronic structure and magnetic properties such as total spin magnetic moment and Curie temperature of the Mn_2-X-Sb (X= Co, Fe) inverse Heusler alloys. In this study, the WIEN2k package has been used to perform first-principles calculations based on Density Functional Theory (DFT) and Full-Potential Linearized Augmented Plane Wave (FP-LAPW) method. We have used Generalized Gradient Approximation (GGA) and Local Density Approximation (LDA) to calculate electronic structure and total spin magnetic moment for both alloys. In addition, Tran and Blaha modified Becke-Johnson (TB-mBJ) potential is used to predict the band energy gap in more accurate. The electronic structure calculations reveal that Mn_2-X-Sb (X= Co, Fe) alloys behaves as half-metallic ferromagnetic in nature. The equilibrium lattice parameter of Mn_2-X-Sb (X= Co, Fe) alloys are 5.98 Å and 5.99 Å, respectively. The magnetic moments of both alloys are $4\mu_B$ and $3\mu_B$, which is in good agreement with the well-known Slater-Pauling Rule: $M_t=Z_t-24$. These both alloys are possess 100% spin polarization at Fermi level will making them one of the best candidates for spintronic device applications such as spin injectors, Magnetic Tunnel Junctions (MTJ), spin valves and Spin Torque Transfer-Random Access Memories (STT-RAM).

Keywords: Half-Metallic Ferromagnetism; First-Principles Calculations; Spintronics

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ACCMS-ICMG-011 ***P-03***	M.J.SWAMYNADHAN	Hydrogenation Of Quinoline To 1,2,3,4-Tetrahydrquinoline Using Metallic Clusters Supported By Carbon Based Low Dimensional Materials
ACCMS-ICMG-014 ***P-04***	DR. KAZUHITO SHIDA	A Simplified Method For Irreversible Monte Carlo
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ACCMS-ICMG-030 ***P-74***	DR.THILLAI GOVINDARAJA	First Principles Study On The Dehydrogenation Of Ethylene Diamine Monoborane Adducts And Its Cyclic Products
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ACCMS-ICMG-025 ***P-80***	SREEDEVI GOGULA	Structural, Optical And Luminescence Properties Of Core Shell Heterostructure Cdszn3(PO4)2 Nanocomposite For LED Application
ACCMS-ICMG-127 ***P-81***	SRIDEVI MEENACHISUNDARAM	Magnetoelectric properties of self-assembled close-packed free-standing CoFe2O3 - Pb(Zr,Ti)O3 thin films.
ACCMS-ICMG ***P-82***	Meribah Jasmine J	First principles study of adsorption behaviour of PF_5 gas molecule on S and Mo vacancy MoS_2 monolayer
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FRACMEET-115 ***P-0F3***	VINAY VAIBHAV	Response of Glassy Liquids to Thermal Gradients
FRACMEET-124 ***P-0F4***	UMANG DATTANI	Cavitation transition in pinned glass-forming liquids
FRACMEET-128 ***P-0F5***	PURUSATTAM RAY	Crack growth in heterogeneous environment

P-01: First-principles Identification of Si/Graphite Hetrostructure as Anode Material for Li-ion Battery

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Abstract:

Anode materials require a basic property such as fast and easy insertion of Li and very low redox potential vs. Li+ and to that of the cathode to provide an adequately large battery voltage. According to the Li ion storing mechanism, anode materials can be classified into three categories: (I) alloying (Li alloys with Si, Sn, Ge and Al), (II) insertion (layered structure e.g. graphite) and (III) conversion (CoO_2, FeO_2). Among all anode materials, insertion based anode materials have good electronic conductivity, more safety and excellent rate capability. However, in the insertion based anode material category, graphite is commercialized since inception of LiB's, but has limited specific capacity i.e 372 mAh/g and less stable during de-intercalation of Li ion. Whereas Si alloy is found to be a highly prospective anode material, but the volume expansion during Li insertion is 400 %.

Using First-principles based calculation we proposed silicene/graphite hetrostructure as an insertion based anode material for Li-ion battery, for which the specific capacity is estimated of about 750 mAh/g. Silicene/graphite hetrostructure is stable during Li intercalation and de-intercalation process. We calculated the open circuit voltage for this layered structure. In order to analyze the stability of the structure, formation energy is estimated during Li-ion is intercalated. We also estimated the volume expansion during Li intercalation and de-intercalation process to understand the structural distortion.

Keywords: Battery; Anode; Carbon; DFT; LIB's

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P-02: Study of electronic structure and magnetic properties of substituted T graphene using first principles formalism

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Abstract:

Carbon is a fundamental element of the periodic table which can exist in different forms like graphite (3D), graphene (2D) or carbon nanotube (1D). Among these class of carbon compounds, the Planar T Graphene is a 2D stable tetra ring arrangement of carbon atoms. It has one sublattice per unit cell. Planer T graphene has no linear dispersion like normal graphene. The band structure of planar T graphene is like metal but buckled T graphene is a semimetal with zero bandgap. This buckled Tgraphene band structure has a crossing point near Fermi surface and it shows linear dispersion at п and п ж bands. It is the host of Dirac fermion i.e., T graphene can also sustain the Dirac electrons under a certain pressure without hexagonal symmetry.[1] Introduction of the defect in 2D planar T graphene is important for modifying the electronic structure, band structure, and magnetic properties, transport properties like any other condensed matter systems. Substitution and adatom introduction on planar T graphene sheet can influence the non-magnetic properties of carbons with a different type of hybridization. Using density functional theory (DFT), one can address the problem with substitution and doping of different kind of elements from the periodic table. In our work, we are trying to see how the electronic and magnetic properties change or varying with substitution of elements in T graphene sheet.

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P-03: Hydrogenation of Quinoline to 1,2,3,4-Tetrahydrquinoline using metallic clusters supported by carbon based low dimensional materials

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Abstract:

Benzopiperidine which is known as 1,2,3,4-Tetrahydroquinoline (py-THQ) has been reported to have good cytotoxic nature and can act as an inhibitor for certain malfunctions in cellular signaling such NF-κB, which leads to different types of cancers. Currently many research works are focused on this compound for better understanding and better applications. The direct and most commonly used technique to prepare py-THQ is hydrogenation of Quinoline. But the challenge is due to the other possible hydrogenated products such as 5,6,7,8-Tetrahydroquinoline or decahydroquinoline. Hence the demand for a good catalyst which benefits selective hydrogenation developed the motivation for this work. In this work, we use Density Functional Theory (DFT) calculations to compare the catalytic property of Ni, Co and Ni-Co bimetallic cluster for the selectivity of py-THQ during the hydrogenation of quinoline. These metals clusters are studied in five different carbon based low dimensional environments as (1) metal cluster encapsulated by pure graphene, (2) metal cluster adsorbed on pure graphene, (3) metal cluster encapsulated by N-doped graphene, (4) metal cluster on amorphous carbon, (5) metal cluster adsorbed on N-doped graphene. Our results show that N-doped graphene has better selectivity of the chemical reaction over pure graphene. We will also discuss how reaction mechanism of various carbon based low dimensional environments considered here. This computational approach will guide the experimentalists to find the better catalyst for this selective hydrogenation.

Keywords: Quinoline hydrogenation; DFT; metal cluster

P-04: A simplified method for irreversible Monte Carlo

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Abstract:

Material Genomics is based on advanced Machine Learning (ML) methods, and through its probabilistic foundation, ML can be naturally benefitted from advanced Monte Carlo methods. Markov Chain Monte Carlo (MCMC) is a group of versatile stochastic methods for optimization, integration, and ensemble generation on numerous states in probabilistic models. The states may be a Boltzmann ensemble, or any sequences of events to evaluate the likelihood of a given outcome. Recently, a new type of *irreversible* MCMC methods are under strong interest due to its performance enhancement over reversible (or time symmetric) methods like conventional Metropolis-Hastings (MH) scheme. However, all known irreversible MCMC schemes require an extra care to design the transition matrix, limiting its usage in material sciences. For example, in state-of-the-art irreversible MCMC methods, called “landfill” and “skewed-detailed-balance”, the Hamiltonian of multiple neighbor states are necessary to determine the next stochastic transition, whereas MH requires only 2. To this end, we are now proposing and a new MCMC scheme that offers limited irreversibility but greatly simplified handling of transition matrix. In this report, the proposed method is tested on a small scale 4-state Potts models as a”mock” hard optimization problem that may encountered in actual ML problems. Although this is a preliminary performance evaluation, it is very possible to extend and apply this to general probabilistic modeling in Material Genomics. Of course, direct application of Potts model simulation *per se* can be extended for various target systems.

Keywords: advanced MCMC; Stochastic modelling; Ensemble generation; Optimization.

P-06: Design of Polar Metals in BTO/Metal/BTO Hetero-Structures

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Abstract:

Polar metals are commonly defined as metals with polar structural distortions. Strict symmetry restrictions make them an extremely rare breed as the structural constraints favor insulating over metallic phase [1]. Discovery of Polar Metals in BTO/Metal/BTO hetero-structures with a ferroelectric-like displacement provides a new insight in designing new functional materials [2]. The $BaTiO_3$(BTO), which is a ferroelectric material undergoes transition from centrosymmetric(Paraelectric) to non-centrosymmetric(Ferroelectric) phase with two possible polarization directions of (P+) and (P-). Thus, the three more configurations are possible when a Metallic block is sandwiched between two BTO layers (i,e.) (1) <P+/Metal/P->, (2) <P-/Metal/P-> and (3) <P+/Metal/P+>. In our work, we have considered the metallic block as $CaFeO_3$ where Fe= 4+ ($3d^4$) between two BTO layers. $CaFeO_3$ is metal in Pnma symmetry and charge disproportionate mode (CD) centered at Fe-sites further lowers symmetry to insulating $P2_1$. In this work we will discuss how CD mode can be tuned by various domains with variation of the magnitude of ferroelectric distortion in the BTO region. Our understanding may help us to get to know the new information in designing a new family of polar metals.

Keywords: Polar metals; BTO/Metal/BTO; M-I transition

P-07: Combined Computational and Experimental Investigation on Chemical fixation of CO_2 and catalytic transfer hydrogenation of ethyl levulinate to γ-valerolactone using water-tolerant DUT-series metal-organic frameworks

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Abstract:

In recent years, capture and reuse of carbon dioxide is a major challenge for the human society due to the increase of undesirable amount of CO_2, main constituents among the global warming gases, in atmosphere. Utilizing the captured CO_2 as an efficient carbon feedstock for producing fine chemicals and/or fuel would be very promising for mitigating the global warming. In this work, we propose an innovative concept of chemical fixation of CO_2 and catalytic hydrocarbon conversion to economically efficient biofuel using nano-porous materials such as metal-organic frameworks with the help combined computational and experimental methods. A series of porous metal-organic framework, known as DUT-84(Zr), DUT-53(Hf), and DUT-52(Zr or Hf) (where DUT stands for Dresden University of Technology) were synthesized by using linear 2, 6-naphtalenedicarboxylate as a parent linker. By adjusting the modulator concentration, the connectivity of secondary Building Unit (SBU) can be increased from 6 to 12, which is reflected in different crystal structures possessing **fcu** (DUT-52), **bcu** (DUT-53) and **(4,4) IIb** (DUT-84) topologies, respectively. All synthesized DUTs were characterized with possible analytical techniques and their structural models were initially geometry optimized with Density Functional Theory (DFT). These models are very similar to the reported single crystal structures of the corresponding DUT MOF. Grand Canonical Monte Carlo (GCMC) simulations were employed to predict the strong interaction of CO_2 molecules with the DUT and further compared with the experimental adsorption CO_2 isotherms on DUT at 298K. These highly CO2 selective DUTs were used as the catalysts for atom-efficient cycloaddition of epoxides for producing cyclic carbonates and also the synthesis of gamma-valerolactone (bio-fuel) from ethyl levulinate with isopropanol as the hydrogen source.The catalytic reaction mechanism for cycloaddition reaction of epoxides in presence of CO_2 and catalytic transfer hydrogenation of ethyl levulinate to γ-valerolactone were investigated by using periodic-DFT calculations. The proposed plausible reaction mechanisms followed by experimental studies showed that the 12-connected 3D DUT-52 catalysts exhibited superior catalytic activity to those of the eight-connected 2D DUT-53 and six-connected DUT-84 catalysts.

Keywords: GCMC; CO_2 Conversion; MOF; DFT and Biofuel.

P-08: Impact on the spectroscopic properties of CdO-$FePO_4$ nanocomposites with varying dopant concentrations of V_2O_5

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Abstract:

Typically, cadmium-iron (Cd-Fe) based complex oxides show selectively high sensitivity to ethanol gas over hydrogen, carbon monoxide and isobutene. The iron-based cathode materials, such as $FePO_4$ are attractive for usage in rechargeable batteries because they are low-cost, highly thermal stable, possesses generally good cyclability and environmental friendly. Moreover, among the different transition metals employed as dopants, V_2O_5 is one of the most intriguing elements because of its various oxidation states and different coordination chemistry. Therefore, undoped and V_2O_5 doped CdO-$FePO_4$ nanocomposites are prepared using sol-gel method. The XRD analysis reveals the crystalline and amorphous nature of CdO and $FePO_4$ respectively. Morphological observations using SEM and TEM show the formation of nanoparticles with remarkable morphologies viz., spherical agglomerates and rods. The elemental composition of Cd, Fe, P, Zn, and O are qualitatively obtained from EDAX analysis confirmed the purity of as-prepared nanocomposites and that the chemical composition is close to the starting stoichiometry. The particle size distributions are revealed from TEM analysis. The average crystallite size calculated from Debye-Scherrer's formula collaborated well with the particle size obtained from TEM images. FT-IR spectra showed that PO_4 units existed even in the amorphous matrix of $FePO_4$. The optical band gap considered from diffused reflectance (DR) studies is found to be blue shifted from 1.97-1.70 eV with increasing vanadyl content.

Keywords: CdO; $FePO_4$; V_2O_5; sol-gel method.

P-09: Quenching of magnetic ordering by Nb and Ru doping in $SrCoO_{3-\delta}$ systems

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Abstract:

In this present study, we report on synthesis and magnetic structure of perovskite $SrCoO_{3-\delta}$ samples with partial substitution by Nb and Ru at Co site. All samples are prepared by conventional solid state reaction. XRD shows all the samples are monophasic in orthorhombic structure with I4/mmm space group. Temperature dependent resistivity (ρ) showed linear behaviour above 50 K. However, ρ increased stiffly below 50 K exhibiting Variable Range Hopping (VRH) behaviour. The magnetoresistance (MR) increased with the value of x and reached 35% at 10K with 70 kOe magnetic field. The samples showed ferromagnetic (FM) type transition below room temperature. Saturation magnetization and exchange bias (EB) increases with Nb concentration and the effect is less prominent for Ru doped samples. Different magnetic properties are explained in terms of the valence states of Nb^{5+} and mixed valent $Ru^{4+/5+}$ replacing Co^{3+} by producing Co^{4+} to maintain the overall charge neutrality which induces ferromagnetism. The existence of FM correlated region in antiferromagnetic matrix and irreversible glass state with competing exchange interactions impart the EB effect. The EB value H_{EB} ~7.45 kOe at 10 K is quite significant which might be useful for further technological implementation.

Keywords: Exchange bias; variable range hopping; magnetoresistance

P-10: Computational study of green primary explosive potassium 4,4′-Bis(dinitromethyl)-3,3′-azofurazanate under high pressure.

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Abstract:

The zeal for search of high performance and low sensitive energetic materials is still continuing day by day due to endless demand in both military and civilian sectors. In recent years, several efforts have been taken to predict/synthesis the green primary explosives with desirable sensitivity, high initiative power and enhanced performance to meet the challenging requirements of future primary explosives [1]. The recently synthesized potassium 4,4′-Bis(dinitromethyl)-3,3′-azofurazanate (K_2BDAF) [2] render fast initiating power and high performance detonation characteristics to replace the long standing heavy metal based primary explosives. In the present study, we report structural and electronic properties of the emerging green primary explosives K_2BDAF using first principles calculations as function of pressure up to 10 GPa. We could observe that the dispersion correction methods are important to capture weak intermolecular interactions in order to accurately describe the geometries of the primary explosives. The computed ground state structural properties using optB86b-vdW method are in good agreement with the experimental results. The pressure dependent lattice constants and bond parameters disclose the anisotropic nature and also a sharp discontinuity around 4-5 GPa. Bond parameters analysis revealed that the C-NO_2 energetic functional groups are more sensitive than stable ring structure under hydrostatic pressure. The calculated electronic structure of K_2BDAF using Tran Blaha-modified Becke Johnson (TB-mBJ) potential show direct-to-indirect band gap transition around 5 GPa, which corroborates with aforementioned discontinuity of the structure.

Keywords: Green primary explosives; density functional theory; high pressure studies

Reference

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P-11: Comparative Study of CO_2 Activation on Single Atom Doped Metal Catalysts

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Abstract:

Combustion of fossil fuels, Oil, Coal, Natural gas has increased the atmospheric level of CO_2 in the past few decades. CO_2 is one of the significant greenhouse gas in the atmosphere and is thought to be the main cause of climate change and global warming[1]. Capture and utilization of CO_2 to value added products like hydrocarbons have very little carbon footprint and hence are remunerative. Previous studies of CO_2 adsorption on single-crystal Cu surfaces show that CO_2 is adsorbed more strongly on the stepped surface as compared to the flat surfaces[2]. In the present work Density Functional Theory (DFT) calculations are performed to study the activation of CO_2 via reverse water gas shift reaction. Various facets of copper surface doped with single atom catalyst of alkali metal, alkaline earth metal, and transition metal are studied. Climbing Image Nudged Elastic Bands (CINEB) calculations are performed to determine the transition state energy of dissociation of CO_2 to CO + O. Comparative study for the CO_2 dissociation on flat and step Cu surfaces doped with single atoms is presented with an aim to look for better catalyst that would favor CO_2 dissociation to CO + O which can then be hydrogenated to produce various hydrocarbons like carbon monoxide (CO), methane (CH_4), methanol(CH_3OH), formic acid (HCOOH) or formaldehyde (HCHO).

Keywords: Density Functional Theory, CO_2 dissociation, Activation energy, Copper

P-12: Structural and optical properties of Strontium filled $CoSb_3$ skutterudite

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Abstract:

Among several forms of thermoelectric materials, $CoSb_3$ based skutterudites have garnered much attention for their possible application in automotive waste heat recovery due to its pertinence in mid-temperature range (350 K– 850K). It has a cage-like structure and two relatively large voids which support the phonon-glass electron-crystal strategy. Many researchers have reported on the improved thermoelectric performance by introducing fillers into the voids. In the present study, Strontium filled $CoSb_3$ nanomaterials ($Sr_y CoSb_3$, y = 0.025, 0.05, 0.075 and 0.1) were prepared by Solvo/Hydrothermal method. Powder XRD was employed to investigate the formation of the skutterudite phase and also lattice parameters were determined. The surface morphology was studied by Field Emission Scanning Electron Microscopy (FESEM) and EDX analysis revealed the atomic percentage of elements present in the Sr filled $CoSb_3$. UV-VIS absorption spectrum shows that a single absorption peak was absorbed below 300 nm which is suitable for UV filters and using the absorption peak optical band gap can be calculated. The vibrational modes of both filled and unfilled $CoSb_3$ nanomaterials were discussed.

Keywords: Skutterudites; Nanomaterials; Solvo-/Hydrothermal; Optical band gap; Vibrational modes

P-13: Effect of Electron Irradiation on Surface, Transport and Relaxation Properties of Li Ion Conducting Polymer Composite

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Abstract:

Polymer composite films of Li_2CO_3/PVA were prepared by solution casting method and irradiated with 0-300 kGy at the interval of 50 kGy using 10 MeV electron beam. Various characterization techniques were employed to study the irradiation effect. XPS results shows the atomic ratio of O1s/C1s decreases with increase in radiation dose and this may be due to carbonization as well as changes in the surface chemistry of irradiated samples due to scission/crosslinking of polymer chains, which further changes the physical properties. FE-SEM results showed that the size of the rod like structure decreases with the increase in irradiation dose and is attributed to the formation of covalent bonds between dopant and the polymer results in the enhanced amorphous phase. The AFM results showed the carbonized phase structures separated by potential barriers/conducting islands on the polymer surface consequently the surface roughness increases upto 150 kGy and then decreased for 300 kGy dose. Impedance study shows that at high frequency (from Cole-Cole plot semicircle decreases with irradiation dose) confirms the double layer capacitive behavior within the irradiated sample. The temperature dependence study revealed Li^+ ions mobility and relaxation behavior has been understood and confirms the non-Debye type of relaxation process. Using Wagner's polarization method the transference number has been calculated whose value is found to be 0.994. The existence of single conducting ion species within the polymer was confirmed from the TIC spectra. This study showed the electron irradiation is the best method to modify the physico-chemical properties of the polymer composite.

Keywords: Carbonization; Crosslinking; Chain scission; Mobility; Surface Chemistry

P-14: Photocatalytic activity of Cadmium Sulphide Nanoparticles Synthesized by Hydrothermal Method

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Abstract:

Cadmium Sulphide nanoparticle were synthesized using thiourea and cadmium nitrate by employing hydrothermal route. The nanoparticles are characterized by Raman & FTIR spectroscopy, X-ray diffraction and SEM. The photocatalytic activity of CdS was tested for degradation of Methyl orange. CdS nanoparticles showed high activity for photocatalytic degradation of Methyl Orange.

Keywords: Photocatalyst; FT-IR; XRD; SEM; UV-VIS spectroscopy

P-15: Ultra thin excitonic solar cells from transition metal dichalcogenides

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Abstract:

Two dimensional (2D) monolayers of transition metal dichalcogenides (TMDs) are being extensively studied for last few years, both experimentally and theoretically. They have proved their usefulness in spintronics, optoelectronics, energy harvesting devices and energy storage devices because of their specific electronic, chemical and magnetic properties. In the present work, we present possible potential of TMD 2D monolayers for excitonic solar cell. We focus on two bilayer heterostructure systems, namely $MoTe_2$(2H)/ZrS_2(2H) and ZrS_2(1T)/$ZrSe_2$(1T). These pairs are chosen on the basis of their geometric structures and 2D lattice constants obtained using density functional theory. These 2D TMD hetero bilayered structures have type II band alignment, useful in the process of dissociation of photo generated electron-hole pair into free charges leading to efficient light to electricity conversion. We have investigated the stability of the bilayers from the phonon dispersion spectra. The optical absorption spectra calculated using Bethe-Salpeter (after a single shot GW calculation) indicate absorption in the IR to visible range. These systems have not been studied in literature for their potential application in photovoltaic device like excitonic solar cell. Our study exposes their potential to be used in photovoltaics as ultrathin excitonic solar cell.

Keywords: TMD hetero structure; ultra thin solar cell

P-16: B_2H_6 splitting on catalytic surfaces and role of BH_3 towards hydrogen spillove

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Abstract:

Hydrogen storage under ambient conditions is still a major challenge owing to the difficulties involved in each step of the process. Chemical adsorption of hydrogen has three critical steps: finding the right support (acceptor), the right catalyst to split H_2, and ensuring that once H_2 is split, the H atoms can migrate on the surface with the help of secondary catalysts and eventually hydrogenate the entire material. Although the first two steps are addressed frequently, the third step is still a problem that needs clear understanding and consequently a solution. For this bond-exchange spillover mechanism is effective for reversible storage and release of hydrogen at near ambient conditions. In this work we address these challenges using density functional theory. We show that BH_3, an efficient secondary catalyst, can be produced by symmetrically splitting B_2H_6, on doped metal-free surfaces such as graphene and h-BN as well as on metal organic framework (MOF5). In addition, to reduce computational cost, we develop structural descriptor and predictive model equation to effectively screen potential BH_3 binding sites. Symmetrical splitting of B_2H_6 on different types of materials can address the hydrogen spillover challenge, making efficient storage of hydrogen possible.

Keywords: Hydrogen storage; Catalyst; Descriptor; Density functional theory; Predictive model equation

P-17: Nature of Ag-O Interactions and Prerequisites for Ethylene Epoxidation : Insights from Periodic Density Functional Theory

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Abstract:

Surface-adsorbate interactions are crucial variety of phenomenon at interfaces. Owing to their great utility in understanding of heterogeneous catalytic reactions, these type of interactions are critical for enhancing industrial chemistry. Inherent complexity of such systems demands utilization of a wide array of tools for satisfactory understanding of processes. One of the most important tool is DFT based ab-initio modeling of metal surfaces. Chief advantages of this computational approach is in obtaining reliable electronic data of possible intermediates. Here, we employ same method to Ag(100) facet to further understanding of ethylene epoxidation. Great industrial significance of this reaction systems from increasing demand for ethylene oxide (EtO) and the cost of ethylene (Et). Silver is the most promising catalyst for Et epoxidation reaction. Modern industrial Ag-based catalyst achieve ~90% selectivity towards EtO though it is thermodynamically unstable. This is possible only due to the unique kinetics of Ag catalyst. Our investigation focuses on Ag-O interactions in which we understand nature of Electrophilic oxygen (O_{ele}) and nucleophilic oxygen (O_{nu})[1]. These species in traditional narrative hold great importance, especially O_{ele}, which has been proposed as species involved in direct epoxidation. We further monitor behavior of ethylene with respect to these surface species[2].

Keywords: Ag; ethylene oxide; DFT; epoxidation

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P-18: Investigation of topological properties in 2D cadmium chalcogenide (CdX, X = S, Se, and Te) buckled honeycomb monolayer on substitution of two Cd atoms by Sn atoms.

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Abstract:

Two-dimensional honeycomb monolayer structures doped with tin atoms are designed from (111) surface of cadmium chalcogenide bulk zinc blende structures. On relaxation the buckled honeycomb monolayer shows signature of band inversion between Sn-p and Cd-s orbital at the Γ point. The band inversion stays even with inclusion of Spin orbit coupling (SOC). With the help of first principles calculation within density functional theory and calculation of phonon spectra, we confirm the stability of the system. We have calculated topological invariants, analyzed edge state properties of systems in a ribbon geometry and has studied their band arrangments. Such system may be useful for technological application in Spintronic domain.

P-19: Promoting reactivity of Graphene based catalysts with doping of Boron atom: A roadmap to achieve LH mechanism for CO oxidation

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Abstract:

One of the major challenges faced by the catalytic industries is to imitate the Pt based catalysts with cost effective and highly active alternatives following LH mechanism for the oxidation of CO. In this regard theoretical and experimental studies have done on metal based catalyst (Pt, Pd), metal oxide based catalysts (AuO_2, TiO_2), single atom catalysts (Al, Si, Pt doped graphene) which could follow LH mechanism. The answer to these questions can be only achieved by designing an efficient and low cost novel metal free catalysts for low temperature oxidation of CO following LH mechanism and maintaining less CO poisoning. In this work we carry out density functional theory to study how the incorporation of B atom on graphene nanoribbons (GNRs) can modify the catalytic activity of the surface and we observe that B-doped GNRs are able to bind CO, and the preferred mechanism switches from ER to LH for CO oxidation. DFT results reveals that the doping of AGNR with B atom is energetically favorable for both O_2 and CO molecule adsorption. So the design of catalysts to achieve the efficient pathway for LH mechanism should be done by considering Boron atoms as a primary dopant and nitrogen as a secondary dopant. Increasing the concentration of single N doping will increase the probability of ER rather than LH. The possible reaction mechanisms (LH- Langmuir Hinshelwood and ER- Eley-Ridel), energy barriers, corresponding active sites and stationary points along the CO oxidation reaction are discussed.

Keywords: Adsorption; Oxidation; Metal free Catalyst; Activity

P-20: Stress Wave Propagation in Ferromagnetic Shape Memory Alloy Polymer Composite

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Abstract:

Ferromagnetic Shape Memory Alloy (FSMA)/Polymer composite establish potential acoustic energy absorbing nature than Terfenol-D due to the presence of twin boundary motion. In this study, we have simulated the vibration absorbing nature of the FSMA/Polymer Composite using MATHWORK. For the analysis, longitudinal stress waves were propagated into the FSMA/Polymer composite sample with the assist of piezostack actuator and observed using the PZT sensor. Stress waves propagating through the test sample undergoes reflection and transmission continuously at the boundaries. These continuous, back and forth propagation interferes with each other and produce a resonance. Thus increases the stress amplitude of the sample thereby inducing the twin boundary motion, when stress amplitude is greater than the twinning stress. Thus the stress waves generated from piezo stack actuator gets damped at the twin boundary region. Viscoelastic nature of the polymer also suppresses the certain amount of energy applied. Analysis clearly demonstrates that the transmission of the stress waves from the piezo stack to the FSMA/Polymer sample are limited by the inelastic twin-boundary motion and anisotropic tetragonal martensitic phase nature of the FSMA sample.

Keywords: FSMA/Polymer composite; Stress Waves; Twin Boundary Motion

P-21: Spin transport properties of COFeCrAl/GaAs/CoFeCrAl through first principle calculations

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Abstract:

Half metallic ferromagnetic materials have applications in spintronic devices because of their high spin polarization[1]. Spin gapless semiconductors belong to the class of half metals that have fully spin polarized carriers at the Fermi level so that they exhibit large magnetoresistance and low spin relaxation (Gilbert damping)[2]. Here in we report the electronic structure, magnetic exchange coupling properties of LiMgPdSn-type spin gapless CoFeCrAl material through First principles calculations. Also, CoFeCrAl/ GaAs/CoFeCrAl magnetic tunnel junction is constructed and its spin transport properties are calculated based on the density functional theory combined with non-equilibrium Green's function methods as implemented in QuantumATK package[3,4].

Keywords: Spin gapless semiconductors; Tunnelling magnetoresistance; spintronics

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P-22: Electronic descriptors and design principles of graphene based electrocatalyst for OER using QM/ML approach

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Abstract:

The optimal electrode catalyst for speed-up the oxygen evolution reaction (OER) is a key aspect in renewable energy technologies such as metal-air batteries and fuel cells. The binding of O atom with the catalyst surface plays a major role to describe the overpotential for OER. A descriptor-based approach to identify the best catalysts will simplify the tedious task of experimentally synthesizing and testing all possible combinations of catalysts. With rising interest in sp^2-based carbon materials as catalysis, it is desirable to understand electronic properties to define OER activity. Using QM/ML approach, we proposed π–electronic descriptors and developed predictive models using simple fits, multiple linear regression and random forest regression to identify the best active site of heteroatom (S, P, SO_2, PO_2) edge-doped graphene nanoribbons. Hence, these approach can help to understand physical insights across wide material space towards the search and design of efficient carbon based electrode catalyst for OER through improving predictive capability and reducing the computational cost.

Keywords: OER; carbon; adsorption; fuel cell; electrocatalyst; DFT

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P-23: Investigation of Structural, Electronic, Magnetocaloric properties of A-Site doped La_2NiMnO_6 for Environmental Friendly Refrigeration

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Abstract:

The structural, electronic and magnetocaloric properties of A-site doped double perovskite La_2NiMnO_6 (ALNM) were studied via theoretical and experimental procedures. A large indirect bandgap in both spins states with ferromagnetic property has been observed in ALNM as an effect of spin polarization. XRD revealed Pbnm orthorhombic symmetry with $P2_1/n$ configuration and VSM results showed the T_C of ALNM is around 297 K indicates well ordering of $Ni2^+/Mn^{4+}$ cations and strong exchange interactions. The entropy changes associated with magnetic phase transitions were determined using magnetization measurements in between 270-325 K. The chemical stability, ferromagnetic insulator with high T_C near to room temperature makes ALNM a potential candidate for solid state room temperature magnetic refrigeration.

Keywords: Double perovskite; Magnetocaloric effect; Magnetization; Density of states (DOS)

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P-24: Effect of Electronic Coupling on Charge Transport across Molecular Junctions

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Abstract:

Understanding the charge transport across molecular junction where the molecule is sandwiched between two electrodes is fundamental aspect in molecular electronics. The charge transport across this kind of device depends not only on the testbed architectures but also on the molecule-electrode coupling or coupling strength which helps us to modulate device properties and understand the relation between coupling strength and transport mechanism. Here, we describe several transport models understanding charge transport across Bacteriorhodopsin molecular junction whose I-V data were measured using Conducting Probe Atomic Force Microscopy (CP-AFM) under various illuminations and forces applied at AFM tip. Transition voltage between tunnelling and field emission was found by using Transition Voltage Spectroscopy (TVS). Using TVS, we also found transport parameters such as energy barrier and conductance. Law of Corresponding States (LCS) represent universal I-V curves plotted for reduced quantities. The values of energy barrier and conductance were found by LCS model under various illuminations and different forces applied at AFM tip. Landauer fit is another method useful in finding measure of coupling strength between molecule and electrodes along with transport parameters such as energy barrier, conductance and voltage division factor. These methods revealed that the electron transport across Bacteriorhodopsin molecular junction alters with the change in the coupling strength for dark and various illumination conditions because there is no significant change observed in the energy barrier values where as both the coupling factor and energy barrier play role in altering the charge transport across this molecular junction under various forces applied at AFM tip.

Keywords: Metal-molecule interfaces; Electronic coupling; Transport models; Molecular Junctions

P-25: Understanding catalytic activity of CoPt alloys as function of composition in DFMCs : A first principles investigation.

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Abstract:

In the last few decades, Direct Methanol Fuel cells (DMFCs) operating at low temperatures using methanol as fuel are believed to be an important source for production of electricity because of lower emissions combined with higher conversion efficiency[1]. Methanol as a fuel is offering greater promise than many other conventionally used fuels like Ethanol. And hence, Niti Aayog recently recommended the use of Methanol mix fuels for passenger vehicles[2]. However, to become commercially viable, DMFCs must overcome the serious limitations of the extensively used Pt-based catalysts. High cost, poisoning due to CO and deformation due to particle agglomeration[3] being the major issues. For the same purpose, alloying of Pt with one of the transition metals (Cu, Rh, Co, Ni, Ir) is being investigated[4]. It is believed that in the Pt-M (M=transition metal) systems the metal atoms help in lowering the d-band center and hence enhancing the catalytic activity. It has been shown both theoretically and experimentally that the Pt-M systems perform better than pure Pt catalysts[5]. In this work we present a DFT investigation of the catalytic activity of Co_xPt_{1-x} (x=0, 0.25, 0.5, 0.75) systemss. It has been observed that $Co_{50\%}Pt_{50\%}$ is the best in stabilizing an incoming methanol molecule. The significant lowering of d-band center of Pt atoms (active adsorption sites) in this case is the main indicator of enhanced activity for this particular composition. We further also investigate the performance of Co_xPt_{1-x} clusters to understand finite size effects on the reactivity of the alloy.

Keywords: Methanol Fuel Cells; DFT; CoPt

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P-26: Detection of Toxic Phosgene gas on highly active Boron Centered Carbon Allotropes : First Principles Study

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Abstract:

Phosgene (COCl2) is extremely toxic and colourless gas and its odor is similar to freshly cut grass. It is a severe lung irritant, and can cause pulmonary oedema, asphyxia and even death at a concentration as low as 2 ppm. The colourless gas is not noticed easily when inhaled, and, more dangerously, its irritant effect does not appear immediately after exposure to fatal levels it has been used as a chemical weapon in World war I because of its highly toxic nature. Phosgene is widely used in industries especially for the production of urethanes and polycarbonate plastics, Therefore, developing a simple and sensitive method for phosgene detection is highly desirable not only for industrial production but also for public safety against terrorist attack. Using first-principles method we proposed Boron doped carbon allotropes such as Graphdiyne, Pentagraphene and Phagraphene as a Phosgene gas sensor. In order to analyze the stability of Boron doping with different carbon based structure the formation energy is estimated. We investigated and discuss about the adsorption of highly toxic Phosgene (COCl2) gas on the Boron doped Graphdiyne, Pentagraphene and Phagraphene. The adsorption energy, partial density of states (PDOS), work function and charge transfer mechanism i.e., charge density difference, planer average charge density difference, Lowdin charge, along with this sensitivity, selectivity, recovery time and the effect of Humidity and on the doped carbon allotropes is discussed in detail. Overall we demonstrate that the surface modification can change the inert carbon allotropes into highly active sensor materials.

Keywords: Adsorption; Carbon materials; Sensors; DFT

P-27: Coexisting topologically insulating and thermoelectric phases via strain engineering in $MAPbI_3$ topological insulator (MA = CH_3NH_3): A first principle study

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Abstract:

Many of the topologically non-trivial insulators are found to be thermoelectric materials due to the presence of heavy elements and narrow bulk band gaps. This investigation is done so as to study the impact of strain on the thermoelectric properties of a topological insulator perovskite material $CH_3NH_3PbI_3$ utilizing first principle based DFT calculations. Initially the calculations have been performed for evaluating the structural relaxation and electronic band structure. Further the transport properties have been calculated by using BoltzTRaP code. It is found that the thermoelectric figure of merit gets slightly enhanced upon compression (positive). The computations are been performed for $CH_3NH_3PbI_3$ perovskite in pseudo-cubic phase having spacegroup *Pmm-3* by varying lattice constant from 6.4 Ȧ (ground state) to 6.3 Ȧ, 6.2 Ȧ, 6.1 Ȧ , 6.0 Ȧ, 5.95 Ȧ, 5.9 Ȧ, 5.85 Ȧ, 5.8 Ȧ. The previous strain study of $CH_3NH_3PbI_3$ indicates that it is strong topological non-trivial insulator at lattice parameter 5.8 Ȧ. In this work the maximum figure of merit observed is 1.12 for lattice constant 5.8 Ȧ at 800K. Thus the present study indicates that $CH_3NH_3PbI_3$ preserves its thermoelectric behaviour along with nontrivial strong topological insulating phase transition after certain strain amounting to 9.1 GPa pressure.

Keywords: First principle study; Thermoelectric; Perovskite

P-28: *Ab-initio* study of novel intermediate band solar cell materials: $ZnSi_{(1-x)}M_{(x)}P_2$ (M=Ti, V)

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Abstract:

Solar energy harvesting is primarily done by converting it into electrical energy through solar cells. Majority of solar cells on the markets are fabricated using single-band gap materials(Si,GaAs). These materials are transparent to lower energy photons thus being unable to tap energy from these energy ranges. But, with the introduction of the intermediate band between valence band and conduction band, the lower energy photons can be absorbed by the modified material thus increasing the efficiency of the solar cells based on them. Cells based on these materials could reach up to 63.2% efficiency theoretically. Among such materials, Chalcopyrite-based materials are currently one of the most promising candidates for intermediate band solar cells (IBSCs). Here, we report that $ZnSi_{(1-x)}M_{(x)}P_2$ (M=Ti,V) could be a promising candidate for being an IBSC. In our investigation, the calculations are based on density functional theory, employing the generalized-gradient approximation for exchange-correlation terms and focusing on the band structure, density of states and the optical absorption spectrum. From the band structure analysis it is found that, intermediate band forms when a single transition metal atoms is substituted into the Si site of $ZnSiP_2$ supercell. From the density of states it can see that the half-filled intermediate band is formed by the M-3d state. Lastly, from the orbital absorption spectrum, it can be inferred that $ZnSi_{(1-x)}M_{(x)}P_2$ can absorb the lower energy photons when compared to Si's absorption; having better absorption in the range between 0.65 to 2.1 eV. Our *in-silico* results predict that $ZnSi_{(1-x)}M_{(x)}P_2$ is a potential IBSC.

Keywords: Solar cell materials; Intermediate band solar cell material; Density functional theory

P-29: An inside into Photoluminescence property of colloids of Zn-Fe Layered double hydroxide.

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Abstract:

Carbonate intercalated ZnFe LDH was synthesized and unexpected photoluminescence of its colloid in formamide was reported. LDH nanoparticles were fabricated by a simple and cost-effective co-precipitation method at constant pH(10) followed by hydrothermal treatment. Prepared LDH was characterized for structural studies by XRD and FTIR. XRD results confirms rhombohedral phase. FEG-SEM showed platelet like structure and particle size evaluated by TEM was about 5-6nm. EDX provides details of elemental composition of Zn-Fe LDHs. A laboratory investigation was done to study the Photoluminescent ability of colloids of ZnFe LDH. Colloids were prepared by delamination of pristine LDH in formamide at room temperature. The generation of surface defects during delamination was believed to be the reason for Photoluminescence. Also, the dependency of Photoluminescence on concentration of LDHs nanoparticles in colloids was studied. Excellent PL property of ZnFe LDH colloids is expected to show the potential applications in the optical field of LDHs.

Keywords: LDH(Layered double hydroxide); Photoluminescence; colloids; coprecipitation; delamination

P-30: Excellent energy density and dielectric properties of ZnO reinforced PVDF/ $BaTiO_3$ nanocomposite

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Abstract:

In this paper, we report the ZnO well synthesized by solution chemistry method and then reinforced with PVDF/$BaTiO_3$ nanocomposite. Piezo-ceramic composite successfully synthesize by spin coating method and characterize by XRD, SEM, EDS and FTIR techniques, which confirm the structure, crystal plane and morphology of composites. The maximum energy density of composite was found to be 0.027 J/cm^3 at 6 MV/m with 78 % harvesting efficiency. Maximum dielectric constant is 1110 at 1 Hz for P-BT-ZnO_f nanocomposite. These results provide a potential way to enhance the performance of composites for energy storage, capacitors, transducers, sensors, etc.

Keywords: Piezoelectric 1; Dielectric loss 2; Energy harvesting efficiency 3; Ceramic 4

P-031: Electrolytic Solvation effects in Fluoroethylene carbonates and Trifluoropropylene Carbonate: A comparative study based on first principles calculation

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Abstract:

Due to the high energy/power density, high specific capacity and low self-discharge rate, Li-ion battery (LIB) has been implemented in wide area of applications starting from small electronic devices to large electric vehicles. However, the use of LIBs in electric vehicles have still not commercialized in large scale due to the unavailability of electrolytic solvents for high voltage LIB. Recently, fluorinated carbonates especially fluoroethylene carbonate (FEC) and trifluoropropylene carbonates (TFPC) have gained much attention as the high voltage electrolytes for having desirable physical properties such as low melting points, low flammability, and high electrochemical stability. Although, the solvation properties of Li^+ in both electrolytic fluorinated carbonates solvents require detailed investigations. With the first principles calculations and polarised continuum model, present work provide the comparative study of structural, electronic and solvation properties of Li^+ solvated by FEC and TFPC i.e. Li^+-$(FEC)_n$ and Li^+-$(TFPC)_n$ where n=1 -5. Our investigation found the solvation number four for both cases, which shows excellent agreement with experimental result. Furthermore, we have found that structural properties, e.g., bond length and associated IR frequency and further Mullikan charge show similar variation for both fluorinated Li-carbonate complexes. However, comparative higher value of solvation energy and lower value of the desolvation energy for Li^+-(TFPC) complexes than Li^+-(FEC) complexes suggest that TFPC could be a better electrolytic solvent for the high voltage LIBs.

Keyword: Li-ion Battery, Fluorinated carbonate; electrolytic solvents; solvation energy

P-032: First principles investigation of silaboranes (SiB_nH_{n+1}; n=4 –13) as potential electrolyte in lithium-ion batteries.

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Abstract:

With the increasing interest in developing high voltage Li-ion battery, it is essential to design and fabricate suitable electrode materials and electrolytes. Most of the commercially used electrolytes consist of organic solvents, which are toxic and highly sensitive to thermal aberrations. The Wade-Mingo's rule obeying monovalent super-halogen electrolytes such as carboranes (CB_nHn_{+1}) and silaboranes (SiB_nH_{n+1}) have recently been reported for their application as high voltage electrolytes in Li-ion battery. As larger anions allow for improved mobility of the Li^+, thus silaboranes can provide an effective solution as electrolytes that could provide both stability and improved energy density to the li-ion system. However, to analyse the intrinsic electrochemical characteristics of silaboranes, precise study at atomic level is required. Therefore, taking help of the first principles based density functional theory, we have investigated the electronic structures of the silaboranes (SiB_nH_{n+1}; n=4 to 13) including their interaction with Li-ion. The decrement in binding energy of the complex, $LiSiB_4H_5$–$LiSiB_{13}H_{14}$ (from 5.92 eV to 5.02 eV), with increase in the ionic size shows low stability, i.e., high efficiency. We have also calculated the HOMO – LUMO gap, which shows that with the increase in the size of the silaboranes, the gap goes on increasing corresponding to the decrease in stability. This is in good agreement with the previously reported theoretical models. The details of the analyses carried out in this work have been explained on the basis of perturbative stabilization energy, charge transfer, vibrational spectra and availability of maximum states.

Keyword: SIlaboranes; Li-ion battery; HOMO-LUMO gap; Energy density; Binding energy

P-033: A DFT study on electronic structure of Cr doped pristine and doped MoS_2 multilayers

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Abstract:

Injecting spin polarised electrons from a ferro-magnetic electrode to semiconductor in Magnetic tunnel junction devices is a great challenge. Doping of magnetic impurity in semiconductor can drastically alter materials properties and may introduce Ferro-magnetism leading to a Dilute magnetic semiconductor which has greater spin lifetime, thereby enhancing injection of spin polarised electrons from the ferro-magnetic to the semiconductor. Molybdenum disulphide (MoS_2) is one of the layered transition metal Dichalcogenides (TMDC) and shows exceptional electronic properties and possible candidate material for spintronic devices. Transition metal Cr doped pristine and multilayer MoS_2, their stability, electronic and magnetic properties are studied using ab-initio based Density functional theory method. Possible in-plane and out plane configurations are considered for the dopants to determine the lowest energy structure and optimal distance between the impurity atoms. The Density of states and band structure for doped as well as undoped bulk and multilayers shows different properties with layer thickness. The doped Cr atoms energetically prefer to stay at nearest neighbour distances by forming a two atom defect complex. The C_{3v} symmetry of the bulk MoS_2 is broken in Cr doped systems due to Jahn-Teller distortion leading to semiconducting nature of the doped systems.

Keywords: MoS_2; Diluted magnetic semiconductor; Density functional theory

P-034: Dip and Dry Coated MWCNT Thinfilm as Counter Electrode in Dye Sensitized Solar Cell.

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Abstract:

Simple and cost effective chemical route, has been used to assemble Dye Sensitized Solar Cell (DSSC). ZnO thinfilm as photoanode was deposited by Successive Ionic Layer Adsorption and Reaction (SILAR) for seed layer of ZnO and Chemical Bath Deposition (CBD) for nanoporous layer of ZnO. Eosin-Y dye and Iodine tri-iodide has been used as dye and electrolyte respectively. Simple and easy, dip and dry deposition method has been used to prepare Multi-walled carbon nanotubes (MWCNT) thin film as Counter Electrode (CE). Number of deposition layers was increased in order to study the effect on the efficiency of DSSC. Structural and Electrical properties were studied using XRD, FTIR, FESEM-EDAX, IV and QE. FESEM showed fibrous and non-distorted structure of MWCNT even after deposition. Maximum power conversion efficiency of 0.29% was obtained for 18 layer of dip and coated MWCNT under 1 sun (AM 1.5G, 100 mW/cm^2). Quantum Efficiency was observed to be nearly 12%.

Keywords: Dye Sensitized Solar Cell; Dip and Dry; Counter Electrode; MWCNT.

P-035: Developing Guiding Principles for Designing Improved Catalysts for Ammonia Borane Dehydrogenation using Density Functional Theory

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Abstract:

Increasingly growing global energy demand has urged the discovery of novel materials that can address these challenges by employing existing technologies. Traditional fuels generally lead to high carbon-emissions which have been a threat to the environment. Hydrogen has evolved as one of the most promising sustainable energy resources due to its high energy density and environmentally clear nature within the fuel cell technology. A longstanding challenge is to store hydrogen on-board because of its low-density. Although ammonia-borane (AB) has emerged as a mainstream on-board H_2 storage material due to high H_2 content, its commercialization remains difficult due to its poor dehydrogenation kinetics. Taking this into account, our work focuses on a computational approach to examine existing dehydrogenation catalysts (such as ruthenium-based catalysts) to develop guiding principles that can used for designing and screening improved catalysts for AB for dehydrogenation.

Keywords: H_2 storage; Ammonia-Borane; Dehydrogenation; Catalysis; Density Functional Theory

P-036: Simple and template-free fabrication of one-dimensional nickel phenylphosphonate nanorods and their calcined derivatives as an advanced electrode materials for energy storage application

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Abstract:

A highly uniform porous 1-D nickel pyrophosphate (PNP) nanorods have been developed by a simple and green approach for the first time and served as excellent electrode materials for energy storage application. The as-prepared materials were characterized by XRD, FE-SEM, HR-TEM and cyclic voltammetry methods. The PNP materials have demonstrated good performance in capacitance, with a higher specific capacitance of 1517 F g^{-1} at 0.5 A g^{-1}, good capacity retention (58%) at 5 A g^{-1}, and excellent cyclic stability up to 3000 charge-discharge cycles (81.5%).

P-037: A Survey on Continuous Control with Deep Reinforcement Learning

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Abstract:

The advent of reinforcement learning was marked by providing simplistic solution to some challenging problems in robotics and decision making strategies [1]. This was proved by beating humans in Chess, Backgammon, and most recently in Go [2]. With the milestone of handling higher dimensional visual data for continuous control, reinforcement learning started to gain confidence in various applications, such as robotics, autonomous driving and energy management in microgrids. In this restricted survey, we shall discuss its implications towards making autonomous robots which promises more robustness compared to the present-day algorithmic ones. After introducing the value-based and policy-based methods, we shall proceed to how this topic branched into different avenues, and how researchers overcame the curse of (a) dimensionality, (b) real-world samples and (c) goal specification. Our survey will cover state-of-the-art algorithms including advantage actor-critic, deep deterministic policy gradient, trust region policy optimization and proximal policy optimization. We shall also demonstrate their competitive performance and convergence with different random seeds [3]. In conclusion, we shall mention some current areas of research within this field, including meta-learning and its viable application towards material informatics.

Keywords: reinforcement learning; learning control; policy gradient; actor-critic

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P-038: Electronic Structure Studies of Bare and Passivated Cadmium Telluride Cages with Fe/Co Doping

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Abstract:

We report on electronic structure studies of a semiconducting stoichiometric cage-like Cd_9Te_9 cluster. As there is reduction in coordination number from bulk form to cluster, the cluster exhibits dangling bonds. These unsatisfied bonds keep the cluster chemically reactive and result in unstability of the cluster. Also the states due to such dangling bonds appear in the energy band gap region, which leads to false estimation of gap or nature of nanostructures. There are substantial changes in the electronic structure of the cluster on passivation with fictitious hydrogen like pseudo atoms. In particular, a widening of the energy gap between the highest occupied molecular orbital (HOMO) and the lowest occupied molecular orbital (LUMO) energy levels is seen, accompanied by an increase in the binding energy per atom in the cluster. Passivation shifts the states due to dangling bonds to far above the LUMO and below the HOMO levels.

Bulk CdTe is half metallic when doped with certain transition metal (TM) atom. When the bare cluster is substitutionally doped with 3d transition metal atoms (Fe and Co), the cluster is found to retain its semiconducting nature whilst passivated cluster is half metallic in nature. A comparison of the atom projected density of states corresponding to bare and passivated clusters on doping with transition metal atoms suggests that the half-metallic nature can arise due to p-d hybridization in the cluster. The suitability of the cage-like cluster for spintronics applications will be discussed.

Keywords: Half metallic; Spintronics; Passivation

P-039: Structural, Electronic and Optical properties of $Sn_9O_5Cl_4(CN_2)_2$ using density functional theory

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Abstract:

The tin carbodiimide compound $Sn_9O_5Cl_4(CN_2)_2$ was recently synthesized by Löber et al[1]. We study the structural, electronic and optical properties of the compound using density functional theory as implemented in VASP [2]. The compound crystallizes in the orthorhombic space group $C222_1$. The structure consists of a $[Sn_8O_3]$ cluster, with Sn atoms forming the motif of a hexagonal bipyramid. Another tin atom and two oxygen atoms connect these clusters into chains. Electronic structure and optical studies reveals that the material is an indirect band gap semiconductor with a wide bandgap.

Keywords: density functional theory; tin carbodiimide; electronic structure;

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P-040: Density functional study of structural and electronic properties of ternary transition metal sulphides MAS_3(M ≡ Hf, Zr; A ≡ Pb, Sn)

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Abstract:

Ternary transition metal sulphides MAS_3(M≡ Hf, Zr; A≡ Pb, Sn) are compounds that crystallizes in the orthorhombic space group PNMA (62) [1][2][3]. We study the structural and electronic properties of these materials using Density functional theory using different exchange-correlation functionals as implemented in VASP [4]. Structural studies show that the MAS_3 type compounds are iso-stuctural with similar lattice parameters. The electronic structure studies reveal that the materials are semiconductors with band gap ranging from 0.9 eV to 1.5 eV. The band gap range of these materials suggests that these materials are good candidates for photo voltaic applications.

Keywords: Density functional theory; Ternary transition metal sulphides; Electronic structure;

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P-041: Tamm states in Topological Insulator – Photonic Crystal Structure

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Abstract:

Topological insulators are quantum materials that have an insulating bulk state and a topologically protected metallic surface state with fascinating electronic and optical characteristics. Surface plasmon polaritons (SPPs) were observed in topological insulators such as Bi_2Se_3, Bi_2Te_3 and $Bi_{1.5}Sb_{0.5}Te_{1.8}Se_{1.2}$ (BSTS) in ultraviolet, visible, and infrared spectral regions. We present tunable Tamm plasmon polaritons (TPPs) in a composite structure consisting of BSTS and one dimensional photonic crystal (1DPC). The dispersion characteristics and the most efficient excitation conditions of TPP mode has been explored using transfer matrix method.

Keywords: topological insulator; Tamm plasmon polariton; photonic crystal

P-042: Family of two-dimensional octagonal monolayers.

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Abstract:

With technological advent, extreme interest has been grown on prediction and synthesis of known and new phases of two-dimensional (2D) materials and their versatile applications. Hexagonal family of material dominates this regime. A new class of 2D family of octagonal monolayers (*o*-MLs) has been emerged recently. To this direction, we propose stable *o*-MLs of metal nitride and carbide family (BN, AlN, GaN, GeC, SiC) along with C, BP and ZnO. Such *o*-ML phase can be possible for other suitable materials of group IV, III-V and II-VI. The general properties for stability in *o*-ML form are discussed along with possible mechanism for stabilization. These *o*-MLs are proposed to show partial ionicity because of nhomogeneity in the in-plane hybrid *p*-states bonding of the host material. To the best of our knowledge, this is the first report of showing partial ionic bonding in the *sp*2 hybridized 2D *o*-C allotrope of carbon. Owing to similar lattice parameter and energetically favored substitution of C8 rings, *o*-BN and gapless *o*-C have shown compatibility to form their patterned hybrid assemblies by substitution of C8 rings in *o*-BN. These assemblies can show variation in the band gap and stability as a consequence of atomic concentration of C, inherent partial and induced ionicity of host and dopant, structure and size of C8 rings, and so forth. Based on the understanding of o-ML family, the octagonal ring poses as more fundamental unit building block and can be of interest for energy harvesting, catalytic and optoelectronic applications.

P-043: First Principle Study of Photocatalytic reduction of carbon dioxide using TiO_2/graphene oxide hetero-junction

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Abstract:

Photocatalytic conversion of carbon dioxide to valuable chemicals by using semiconductor materials is the one of the intriguing challenges in materials science. Higher efficiency and product yield can be achieved by designing of a suitable photocatalyst with retarded recombination of photogenerated electron-hole pair and sufficient potential for the reduction of CO2. In this work, using density functional theory, we have designed heterojunction of reduced graphene oxide and anatase TiO2 (001) surface for better photocatalytic reduction of CO2. A finite bandgap appears at the Fermi which is attributed to the graphene-oxide and as result the interface absorbance edge is shifted to visible range. Our proposed model interface provides best commensurate unit cell for the heterostructure with minimal lattice strain. Such a unique structure helped the separation of photogenerated electron-hole pairs with better charge transfer to perform the reduction of adsorbed CO2 molecules. It is earlier reported that the rGO/TiO2 multi-leg nanotubes (MLNTs) have shown the highest photocatalytic activity which agrees with our present work on TiO2-rGO heterostructure.

P-044: Numerical studies of the deformation behavior for Fe-Cu on different length scales

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Abstract:

In the present work, numerical simulations are employed to investigate and correlate the materials deformation behavior for Fe-Cu single/polycrystalline materials on different length scales. In particular, finite element simulations, micromechanical formulations, atomistic simulations and discrete dislocation dynamics simulations have been employed. The reliability of the prediction of the deformation behavior is investigated by comparison with the numerical simulations at different length scales and experiments.

Keywords: Atomistic simulations; compression tests; elasto-viscoplastic material model; micromechanical formulation; discrete dislocation dynamics simulations

P-045: Novel low dense carbon allotropes with tunable band gaps

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Abstract:

Allotropes of carbon are very well known for their diverse structure and excellent properties. Diamond is the naturally occurring hardest elemental material known to the humankind. The graphite and its analogous structures, graphene and graphdiyne are omnipresent and they occupy a pivotal role in the chemistry and physics of contemporary materials. The nanoscience and engineering is spearheaded by fullerenes and nanotubes. In this multifarious carbon kinship, here, we propose different novel carbon networks built based on parental skeletons of carbon allotropes with molecular carbon spacers as linkers. The model structures are calculated for their electronic structure and stability using density functional theory and density functional perturbation theoretical methods. The calculated structures are found to be remarkably stable; the phonon dispersions suggest that the structures are dynamically stable. All the carbon structures studied here with varied densities due to spacers are found to be semiconductors with tunable band gaps. The predicted novel structures, structure-property correlations, and the results of the electronic structure calculations will be presented.

Keywords: carbon-allotropes; diamond; electronic properties

P-046: Electronic Structure, Lattice-Dynamics and Superconductivity in Ag-Au Alloys

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Abstract:

Despite the fact that monovalent noble metals defy superconductivity at atmospheric pressure, it has been proposed recently evidence for room temperature superconductivity at ambient pressure in nanostructures of silver particles embedded into a gold matrix (1,2). The origin of this emergent phenomenon in these Ag-Au nanoalloys is unclear. The alloys may have different chemicophysical interactions (3) leading to the formation of Cooper pair, the bosonic quasiparticle responsible for the superconductivity. To investigate this both in theory and computations, knowledge of the alloy structure is necessary. Therefore, here we predict crystal structures of Ag-Au alloys (3D crystals and 2D slabs) using knowledge and first principles based crystal structure prediction approaches. For the most thermodynamically stable and metastable structures resulted, the superconducting transition temperatures (T_c) are estimated by carefully calculating electronic structure and electron-phonon matrix elements. All the structures investigated are found to be metallic with a common fcc-like cuboctahedron Ag-Au structure motif, featuring similar electronic densities of states near the Fermi surface.

The T_c are estimated within the Bardeen-Cooper-Schrieffer (BCS) formalism; it turns out that in calculations for all the Ag-Au structures we have predicted, the transition temperatures resulted in less than one milli Kelvin (4-6). The BCS calculations do not indicate any sort of room temperature superconductivity as proposed in references 1 and 2, but rather our results complement the observations of near absence of superconductivity in pulsed laser deposited Ag-Au modulated nanostructured thin films (7) and ~2 K in Ag implanted in Au thin films (8). Probably, as proposed (1-3) the superconductivity may be lurking in the domains of the grain-boundaries, may be vindicated in the Fermi-surface topology. Detailed methods, calculations, and results of our investigations will be presented.

Keywords: superconductivity; alloys; electron-phonon

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P-047: Theoretical investigation of charge transport properties in bowl-shaped perylene-derivatives.

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Abstract:

The organic semiconductors (OSCs) take advantages from their unique characteristics like low-cost, ease of synthesis, solution processability and high flexibility. Therefore, the fields of smart electronics like organic light emitting diodes (OLEDs), organic field effect transistors (OFETs), organic semiconductor sensors (OSCSs), and organic photovoltaics (OPVs) are looking for the fast-track practice of the OSCs in the flexible devices. Apart from the easy charge transport property, a persuasive air-stability and good charge injection happen to be the basic requirements of OSC applications. Oligoacenes are the mainstream small organic compounds with π-conjugated planar chain, those have been widely studied in the last few decades, whereas, the low-stability limit their applications in electronic devices. The current interest in the non-planar OSCs has led to the development of several bowl-shaped, helical and saddle-type structures, which have shown improved charge transport property and solubility. Herein, we have studied the charge transport property of a series of bowl-shaped perylene derivatives through density functional theory. The compounds typically show a p-type characteristic, with their highest occupied molecular orbital (HOMO) energy levels lying at ≈5.3 eV, indicating better hole-injection from a typical Au-eletrode (work-function ≈5.1 eV). While, upon increasing the π-conjugation of the perylene backbone, the lowest unoccupied molecular orbital (LUMO) energy level gets aligned towards >3 eV, increasing the chance of electron-injection as well. Such property of these small OSCs opens up the possibility in developing the air-stable, n-type/ambipolar compounds.

Keywords: organic semiconductors; bowl-shaped; perylene; density functional theory

P-048: Effect of Curcumin doping on optical, Structural and luminescent Properties of PVA polymer films

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Abstract:

Over the last several decays the field of polymer composite has undergone an enormous expansion due to its verity of optoelectronic applications. The property of polymer composite depends on both polymer as well as dopant. Thus, we can tune the required properties of polymer by adding suitable dopant. Curcumin doped PVA films with different concentration are prepared by solution casting method to study the effect of curcumin concentration on optical, structural and luminescent properties. FTIR spectra were carried out to identify the role of chemical interface damping which influenced the broadening of the absorption band. The optical properties like, dipole strength, transition dipole moment, dipole length, oscillator strength, the decrease of optical band gap and increase of activation energy with dopant concentration were observed from the UV–Vis study. These doping mechanism may be attributed to the creation of defects and formation of charge transfer complex. The obtained optical parameters were found to be strongly affected by Curcumin dopant. Fluorescence emission spectra consist of broad band at 333 nm for 268 nm excitation and peak shifts towards higher wavelength region with decrease in intensity upon doping. These observations have been correlated to the measured fluorescence spectral features. XRD data revealed structural modification such as increase in degree of crystallinity and it is correlated with morphological nature of these films were observed through SEM results.

Keywords: Curcumin; complex formation; dipole moment; polarization and anisotropy

P-049: Feasibility and Assessment of PCM Based Heat Sink for Self-Powered Devices

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Abstract:

In this study feasibility of a new flexible phase change material (PCM) heat sink is examined. The phase change material has the ability to hold the temperature difference for a long period of time due to its latent heat capacity. The designed heat sink can be reused because the PCM solidifies at room temperature. Moreover, the designed flexible PCM heat sink is small in size and light in weight compared to the conventional metal heat sink with high performance. In order to maximize the power produced by device, the Multiphysics analysis i.e. thermal and electrical interface is studied in detail. At last, to optimize the thermoelectric and heat sink, parameters are defined such as leg length, surface area of thermoelectric generator and height of heat sink. The results help to derive a conclusion on assessment of PCM heat sink integrated with TE device for wearable device with the purpose of optimizing the electrical power while minimizing the total volume. The developed heat sink presumes to bring about commercialization of self-powered wearable devices.

Keywords: Thermoelectric Module; Wearable Heat Sink; Self-Powered Devices

P-050: Theoretical investigations on two dimensional Cs_2TiBr_6/TiO_2 heterostructure for solar cell applications.

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Abstract:

To elevate the efficiency of silicon photovoltaic device, tandem solar cell architecture is a highly desirable strategy. The interfaces in tandem solar cell offer a very exciting research area, which can be explored in order to increase the efficiency of the device. Herein, we studied the interface between the absorber layer (Cs_2TiBr_6) and electron transport layer (TiO_2) using first principles density functional calculations as implemented in Vienna ab-initio simulation package. The calculated band gap values of Cs_2TiBr_6 using PBE and HSE06 functional are 1.51 eV and 1.94 eV, respectively and it is an indirect band gap material. Similarly the band structure of rutile phase of TiO_2 is calculated using both PBE and HSE06 functionals and it has a direct band gap nature with the values of 1.74 eV and 3.09 eV, respectively. In both the cases, band gap values calculated using HSE06 functional is in close agreement with the corresponding experimental value. From total density of states calculations of Cs_2TiBr_6, TiO_2 and its heterostructure, it is observed that the heterojunction thus formed has a typical straddling (Type-I) band alignment. From the absorption coefficient calculations, it is observed that in the visible spectral region, Cs_2TiBr_6 exhibits more absorption coefficient values than heterostructure and TiO_2. Hence, it can be concluded that the photons of visible wavelength range are poorly absorbed in the heterostructure.

Keywords: solar cell material; heterostructure; band alignment

P-051: Microstructural, Optical and Electrical Properties of MoS_2 doped Sodium Alginate.

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Abstract:

MoS_2 doped Sodium Alginate (NaAlg) nanocomposite films were prepared by solution casting method and the prepared nanocomposite films were analyzed using different characterization techniques. From FTIR study, appearance of new peaks and shift in the peaks position indicates the interactions of MoS2 with NaAlg are studied. The optical energy band gap and activation energy is calculated using UV-Visible spectra and is observed that the optical energy band gap decreases and activation energy increases with increase in dopant concentration. Also the change in optical properties like molar extinction coefficient, transition dipole moment, dipole length, dipole strength and oscillator strength are determined. The XRD study shows the increase in degree of crystallinity with increase of dopant concentration, which is attributed to the formation of complex between dopant and the polymer. Surface topography of polymer nanocomposite films was studied using atomic force microscopy (AFM). Here surface roughness increases with increase in dopant concentration, which is in correlation with XRD results due to increase in crystallinity of the nanocomposite films. Dielectric properties of the nanocomposite explain the non-Debye type behaviour. The conductivity occurs due to the easy movement of ions in the polymer matrix after MoS_2 doping, which increases the hopping of mobile ions in the nanocomposite and hence enhancement in the ionic conductivity. Therefore, these polymer nanocomposite films are good electrolyte materials for the fabrication of electrochemical devices.

Keywords: Polymer nanocomposite; MoS_2; Sodium Alginate; Dielectric properties

P-052: A Polymer of Natural Product for Energy Storage in Hybrid Vanadium Flow Battery

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Abstract:

Vanadium redox flow battery (VRFB) is commercially matured system for electrical storage application wherein V^{4+}/V^{5+} redox couple is used as posolyte (*E°=1 V)* and V^{2+}/V^{3+} redox couple is used as negolyte (*E°=-0.26 V).* However, the commercialization of VRFB is limited by the high cost of the vanadium. More than 40 % of the total cost is attributed to vanadium. The uneven geographical distribution and abundancy of vanadium in different countries cause such high cost of vanadium. The ultimate solution is to find out low-cost abundant (irrespective of geographical area) redox materials for aqueous systems. 4,5-dihydroxybenzene-1,3-disulfonic acid (BQDS) and 3,6-dihydroxy-2,4-dimethylbenzenesulfonic acid (DHDMBS) are the only known dihydroxybenzene based aqueous posolyte investigated by S. R. Narayanan *et. al.* which show very high redox potential. However, the cell voltage of assembled battery with those are very less which limits the battery in terms of energy density. In this work we proposed a hybrid flow battery constituting polymer derived from a natural product, dopamine, as postive electrode and V^{2+}/V^{3+} as negolyte. This cell gives an open circuit voltage of ~ 1 V and a capacity of about 275 mAh g^{-1} of polymer.

Keywords: Polymer; dopamine; energy storage; hybrid vanadium flow battery

P-053: Anthraquinone derivative for organic redox flow battery in basic medium.

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Abstract:

Aqueous redox flow batteries are preferred over non-aqueous due to high conductivity of the electrolyte and intrinsic safety associated with it. We have come up with redox flow battery using redox active anthraquinone (anthrarufin) based organic molecule as anolyte and potassium ferrocyanide as the catholyte in basic medium. Anthrarufin shows a maximum solubility of 0.05 M in 1M KOH. The solubility is limited due to the presence of hydroxyl groups adjacent to the quinone group there by avoiding effective solvation by the electrolyte medium. An optimum cell voltage of 1 V is expected from the cell fabricated. The cell shows collection efficiency (CE), voltage efficiency (VE) and energy efficient (EE) of 83%, 87% and 72% respectively at a current density of 20 mA cm^{-2} for 50 mM of anolyte and 200 mM of catholyte. The cell shows rapid capacity fade after 23rd cycle presumably due to the formation of unstable charged species. Naphthazarin (2) and juglone (3) were used for comparative study with anthrarufin. But showed lesser cell voltage as they have poor resonance from 2 benzene ring as compared with anthrarufin having 3 rings. Though (2) and (3) have 2 conjugated aromatic ring, naphthzarin showed lesser cell voltage since it has 2 electron withdrawing hydroxyl groups which increase its reduction potential by increasing LUMO energy level and thereby electronic affinity.

Keywords: Anthrarufin; Potassium ferrocyanide; solubility.

P-054: Binder Free Thin Carbon Fiber Electrode for Vanadium Redox Flow Battery Applications

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Abstract:

Vanadium redox flow battery (VRFB) is emerging as the most preferred energy storage device for the grid and stationary applications. To improve the VRFB power density, one or more of the overvoltages, such as activation, ohmic and concentration polarization(s), in addition to the mass transfer losses need to be manipulated. In this regard, a thin electrode was explored, which consists of a thin layer of graphite felt sandwiched between carbon papers (of 0.2 mm thick each) (CP/GF/CP). The catalyst layer, i.e. graphite felt layer is made of the carbon fibers derived from the carbon felt. Since only a few mg cm-2 of carbon felt is used, there is a greater decrease in the cell polarization leading to improved electrolyte utilization and energy efficiency. Polarisation (I-V) study of assembled VRFB cell with Nafion 117 membrane in 1 M vanadium solution reveals a huge improvement in current density for CP/GF/CP electrode (of about 500 mA cm^{-2} @ 1 V), in comparison to GF electrode (~ 200 mA cm^{-2} @ 1 V). At 100 mA cm^{-2}, the charge and discharge performance of CP electrode-based cell exhibits columbic efficiency (C.E), energy efficiency (E.E) and voltage efficiency (V.E) of 99 %, 86 % and 85 % respectively at the 10th cycle, whereas it is 94 %, 76.6 %, and 81.5 % for graphite felt based one. Hence CP/GF/CP electrode is a potential candidate for high energy VRFB application.

Keywords: Vanadium redox flow battery; graphite felt layer and carbon paper

P-055: Thin Bilayer Micro-Mesoporous Membrane for High Energy Efficient Vanadium Redox Flow Battery

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Abstract:

Nafion, a perfluoro sulfonic acid membrane, is the state of the art separator for the vanadium redox flow battery (VRFB) systems. But, a significant share of the total VRFB cost is attributed to the Nafion membrane. Hence, to cut down the cost thin Nafion membranes could be used. Unfortunately, this move leads to excessive crossover of the vanadium ions leading to capacity loss. In this work we have designed a bilayer membrane wherein, one layer is made of Nafion 212 membrane (50 µm) which has mean pore size of around 2 nm and the other layer is a mesoporous hydrocarbon membrane having a mean pore size of around 150 nm. A 25 cm^2 VRFB assembled using mesoporous hydrocarbon membrane, Nafion 212 and combination of mesoporous hydrocarbon-Nafion212 exhibited a cell resistance of 11, 12.5 and 15.7 mohm respectively. This assembly enhanced the specific capacity of the VRFB running with 1 M Vanadium in 3.5 M sulfuric acid solution from ~ 19 Ah L^{-1} to 22.4 Ah L^{-1} at 100 mA cm-2. Similarly, the energy efficiency was enhanced from 79.8 % to 84.5 % and electrolyte utilization from ~ 73 to 83%. Although the cell resistance of the mesoporous hydrocarbon-Nafion212 combination was nearly 3 mohm higher than that of Nafion 212, the overpotential observed was lower than that of Nafion 212 case. Our interest is to understand why this increment in the specific capacity and energy efficiency has occurred. From the experimental data, it is imperative that the bilayer leads to reduced vanadium crossover thereby enhancing the SOC and specific capacity at any given time during charging and discharging of the VRFB. The VRFB with bilayer membrane delivered peak power of ~ 550 mW cm^{-2} at 700 mA cm^{-2}.

Keywords: Vanadium redox flow battery; vanadium cross over; micro-mesoporous bilayer membrane.

P-056: Molecular engineering of donors and acceptors for tuning the absorption behavior and electron injection for BODIPY based dyes in DSSCs: A computational study

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Abstract:

A series of $(D\text{-}\pi)_2\text{-}A_n\text{-}A$ based organic dyes containing boron dipyrromethene (BODIPY) moiety as an ancillary acceptor (A_n) derivative were chosen. The effect of donor moieties (carbazole, phenothiazine and phenoxazine), and acceptors (benzoic acid, carboxylic acid, cyanoacetic acid, and cyano-phenylacetic acid) was investigated to understand their photophysical and photoelectrochemical properties by employing density functional theory (DFT) and time-dependent DFT. It is proved experimentally that BODIPY enhances the light harvesting in red and near IR region of visible light. The rigidity of donor unit and non-coplanarity between donors and BODIPY moiety influenced the charge transfer properties of the dyes. The electron density distribution analysis was performed for all the dyes to confirm the intramolecular charge transfer, envisioned from the simulated absorption spectra of the dyes. Phenothiazine donor-based dye exhibited the lowest reorganization energy and the highest dye regeneration driving force. The different acceptor units have been screened to tune the lowest unoccupied molecular orbital (LUMO) level for efficient electron injection into the conduction band of TiO_2. Adsorption energies were calculated for different acceptors by varying different modes of binding onto the TiO_2 (1 0 1) surface. Density of states analysis revealed that the absence of defect states in the band gap of TiO_2 facilitates the smooth electron transfer from the excited state of the dye to the conduction band of TiO_2. Considering the LUMO energy level of dyes and conduction band energy level of TiO_2, it is understood that all the dyes studied in this are capable of electron injection upon photoexcitation. Based on the computational studies, pheothiazine donor-based dye would be better suitable dye for DSSC owing to higher dye regeration driving force, lower reorganization enrgy and lower non-radiative decay rate (greater electron injection).

Keywords: BODIPY; DSSC; Dye regeneration; Reorganization energy; TiO_2 (1 0 1) surface

P-057: Impact of various binders and non-precious metal catalyst decorated Ketjen Black carbon as cathode in alkaline zinc-air battery

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Abstract:

Zinc-air battery technology is a stupendous competitor in the automobile sector. Alas, there are a few issues that restrain them from being commercialized. One such prominent issue which has not been discoursed thus far in alkaline zinc-air battery is the impact of the type of binder. The present work incorporates a study conducted to get insights on the impact of ten different polymeric binders in the air electrode of zinc-air battery. The binders under investigation are Fumion, Nafion, PMMA, PVDF, PP, PE, PVP, CMC, Chitosan, PTFE. Herein, the electrochemical characterisations are presented. The Polarisation curves reveal huge variation depending on the type of binder. Nafion ionomer shows a highest current of about 150 mA cm^{-2} at 0.6 V owing to its hydrophobic and conducting nature. This report also involves synthesize of transition metal and nitrogen doped carbon (M-N-C) catalyst, by solid-state pyrolysis by making use of Cobalt (II) tetraphenyl phorphyrin and ketjen-black carbon, named as Co-N doped KBC. The ORR catalyst displayed an Eonset of 0.81 V and a diffusion limited current density of 4 mA cm^{-2}. The as-synthesized material was verified to be a suitable catalyst for primary zinc-air battery with a power density of 50 mW cm^{-2}.

Keywords: Zinc-air battery; Non-precious metal catalyst; Ketjen black carbon; Binder impact

P-058: Magnetism of two-dimensional metallic VTe_2

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Abstract:

Two-dimensional (2D) magnetic materials are highly desired due to their promising applications in atomically thin ultracompact spintronics, on-chip optical communications, and quantum computing. In particular, metallic transition metal dichalcognides (MTMDs) have attracted considerable interest due to their interesting properties, including magnetism, charge density waves (CDWs), superconductivity, electrical conductivity, etc. Recently, the 1T phase of monolayer (ML) VTe2, a typical MTMD, was experimentally synthesized by several groups. Even though earlier theoretical studies predicted 1T ML VTe2 to be ferromagnetic at room temperature, no magnetism was measured in the recent experimental studies. To resolve this discrepancy between theoretical prediction and experimental measurement, we go beyond the currently adopted methods in theoretical prediction of magnetism. The reported CDW state in ML VTe2 suggests many-body effect in VTe2. Therefore, we investigate the magnetic properties of VTe2 by combining the first principle calculation and the renormalized spin-wave theory (RSWT). Results of our study will be reported.

Keywords: VTe2; magnetism; theoretical study

P-059: Recovery of the Dirac states of graphene by intercalating two-dimensional traditional semiconductors

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Abstract:

The epitaxial growth of graphene on transition-metal substrates has proved to be an efficient method to synthesize high-quality large-area graphene. However, due to the interaction between graphene and the transition-metal substrate, the electronic structure of the as-fabricated graphene is distorted. Here, using density functional theory calculations, we investigated the effect of intercalating two-dimensional (2D) silicon and III–V materials, such as double-layer honeycomb AlAs, into the graphene-metal interface. We found that the intercalation of these 2D materials significantly reduces the interaction between graphene and the transition-metal substrate. The Dirac state is largely restored. The doping level of graphene induced by 2D intercalated material and the metal substrate is proportional to the work function difference between graphene and 2D materials/metal. This work provides a way for the formation of freestanding graphene and further fabrication of graphene-based devices.

Keywords: Dirac state recovery; Two-dimensional traditional semiconductors; Intercalation

P-060: Van der Waals hetero-structures of 1H-MoS2 and N substituted Graphene for catalysis of Hydrogen Evolution Reaction

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Abstract:

First-principles theoretical analysis of the catalytic activity of van der Waals hetero-structures of 1HMoS2 and graphene substituted with three chemical types of nitrogen species (i) Graphitic (G), (ii) Pyridinic (Pn) and (iii) Pyrrolic (Pr), for application in catalysis of hydrogen evolution reaction (HER) has been presented. Graphitic and pyrrolic N substituents result in n-type electronic structure, whereas substitution of pyridinic N imparts p-type electronic character to the hetero-structure. Work functions (φ) of the hetero-structures suggest that graphitic N-graphene:MoS2 hetero-structure (φ = 3.8 eV) is expected to be effective in catalysing the reduction of H+ to evolve H2. 1H-MoS2 monolayer in the hetero-structure contributes by enabling increased H2O adsorption and offsetting the band edge energies optimal for the catalytic activity. Near optimum Gibbs free energy of H-adsorption (ΔG+) were obtained for graphitic (ΔG+ ~ 0.29 eV) and pyrrolic (ΔG+ ~ -0.2 eV) N-graphene:MoS2 hetero-structures. Our work showcases how catalytic and electronic properties of the N-doped graphene:MoS2 hetero-structure depends on the chemical identity of N-sites and uncovers a route to 2D hetero-structures with high catalytic activity.

P-061: Effect of impact energy on damage evolution in laminated composite

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Abstract:

In this study, the damage evolution in glass fiber reinforced polymer composites (GFRP) due to low velocity impact is analyzed. A bidirectional GFRP is fabricated by employing hand-layup technique. The laminate is vacuum bagged and cured in a hot press. An ASTM standard D7136M is followed to prepare the test specimens for conducting dynamic experiments. The samples are loaded at seven different energy levels, ranging from 4 J to 30 J. The damage zone, visible at the back surface of the laminates, is observed to increase with increasing impact energy. The fracture energy calculated from the load histories, which are recorded by the data acquisition module of INSTRON 9340, shows that it increases with increasing impact energy. To get more insight into the fracture behavior of the laminates, the samples are carefully sliced at the damage zone and their cross-sections are examined under scanning electron microscope. For all impact energies, a truncated cone shaped damaged zones indicate matrix cracking through-the-thickness. A closer examination reveals that the failure is also accompanied with the delaminations in-between various layers, which increase both in numbers and magnitude with increasing impact energies. At higher energy levels, some of the fibers show fracture around the impact point, whereas fiber-matrix debondings are visible in the rest of the damage zone.

Keywords: Impact energy; damage evolution; fracture; GFRP; delamination.

P-062: Mechanochemical bulk synthesis of CZTSe photovoltaic absorber

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Abstract:

In this work, $Cu_2ZnSnSe_4$ (CZTSe) compounds have been synthesized using ball milling method. This process is cheaper and reliable route for compound material as compared to solid state and hydrazine based solution methods. Structural, morphological, and optical properties of the bulk were studied in detail using X ray diffraction (XRD), scanning electron microscopy (SEM), transmission electron microscope (TEM), Energy-dispersive X-ray spectroscopy (EDS), UV-Vis spectroscopy, and Raman Spectroscopy. CZTSe bulk material was found to have direct optical band gap (E_g) value ~1.0 eV, indicating favorable photoresponse in the visible range of the solar spectrum.

Keywords: CZTSe; photovoltaic; quaternary compound; ball-milling

P-063: Tight Binding Model Study of Centrosymmetric and Non-centrosymmetric Halide Perovskites

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Abstract:

Over the last decade, halide perovskites have attracted considerable attention because of their remarkable photovoltaic applications. The electronic structure plays a vital role in understanding the intriguing properties of these perovskites. In the present work, we have developed a minimum basis set Slater-Koster based generalized tight-binding model, which is applicable for both centrosymmetric and non-centrosymmetric systems. The model is applied to investigate the non-trivial topological phases in centrosymmetric $CsSnI_3$ polymorphs viz, cubic, tetragonal, and orthorhombic phases as a function of biaxial strain and non-centrosymmetric $MAPbI_3$. The variation of effective tight-binding parameters as function strain is presented in the form of an empirical descriptor model, which is capable of predicting the band topology of the halide family. The model consists of a set of linear equations [T] = [D][EC], where [T] represents the set of hopping interactions, D is the family of descriptors specific to a given compound, and [EC] is the externally controlled variables such as the bond lengths and the rotational and tilting angles. Furthermore, the analysis of the band structure reveals that a TB model with the basis set formed out of Sn-{s,p} orbitals of a fictitious cubic Sn crystal is capable of explaining the band topology of $CsSnI_3$ in all of its polymorphs. The model for the non-centrosymmetric systems includes the inversion symmetry breaking term, which is essential to understand the first-order quantum phase transition in cubic $MAPbI_3$ under hydrostatic pressure. While the inversion symmetry breaking field lifts the bulk band degeneracy in the momentum domain, at the surface, it transforms a four-fold degenerate Dirac node into a doubly degenerate Dirac circle along with two doubly-degenerate Dirac nodes one above and one below it in the energy domain. Thus, the present TB model is much more generalized in terms of chemical composition and crystal polymorphs and complete in itself.

References:

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2. Ashish Kore, R. Kashikar, Mayank Gupta, Poorva Singh, and B. R. K. Nanda (Unpublished).

P-064: Experimental studies on mechanical and dielectric properties of liquid-filled dielectric silicone rubber composites

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Abstract:

Silicone rubber possess higher elastic behavior that makes it suitable to be used as compliant material. The low diectric permittivity of silicone rubber limit the usage as compliant dielectric material. Improvement in dielectric properties are achieved at the cost of increased stiffness when reinforced with different solid fillers. In the present study, an attempt is made to achieve higher dielectric permittivity being and also compliance using liquid fillers. Silicone rubber composites are prepared with two different liquid fillers namely Glycerol and Cocos nucifera in three different volume fractions. Dielectric and compression tests conducted on the prepared composites, show improvement in dielectric permittivity with a decrease in modulus. Dielectric permittivity of silicone rubber improved by nearly 72.5% when filled with 15% by volume of Glycerol. For Cocos nucifera composites modulus reduced by nearly 28% with 15% by volume of fillers. The higher ratio of dielectric permittivity to modulus are observed for Silicone rubber Glycerol filled composites, and they could be potential materials for soft dielectric sensors.

Keywords: Silicone rubber; dielectric permittivity; compliant; liquid-filled composite;

P-065: Design optimization on fabrication method of thermoelectric generator module

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Abstract:

In modern life, the world has faced numerous energy crises and overwhelmed by renewable energy sources which also helps to reduce greenhouse gas emissions. In the current scenario, solid-state energy devices such as solar and thermoelectric generation (TEG) technology have more attention for its high-reliability, the establishment in the remote areas, low-maintenance and lightweight. Since solar energy has dis-commodity like capable of power generation during the day time and air pollution levels can influence efficiency, although thermoelectric power generation can avail against surrounding waste heat. To simplify the research and outcome of the practical TEG device on the real condition, this paper proposes a real-time simulation model, consequently the model is divided into three parts: 1) ideal model 2) segmented model 3) hybrid model. The ideal model consisted of bismuth telluride as the p-type and the n-type materials. The segmented and the hybrid models consisted of different combination of materials such as lead telluride and antimony telluride. The optimization of the length of the thermoelectric module was carried out to achieve the highest power output and it was observed to be at 2mm. This paper also investigates the thermo-mechanical stress distribution analysis in the module to find the maximum load the thermoelectric device can withstand before undergoing fracture, depending upon the yield strength of the material. The stress was analyzed in all the three thermoelectric modules and the results are evaluated.

Keywords: thermoelectric module; wearable device; geometric aspect.

P-066: Catalysis on metal flatland decorated Graphene surface

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Abstract:

The novel applications of 2D materials such as graphene have aroused tremendous interest among the researchers. Owing to their properties like high specific surface area and excellent mechanical strength, these materials are of enormous interest in catalysis. Since pristine graphene is inert in catalysis, modifying the graphene framework for tuning the properties of graphene and also to induce the catalysis in graphene is the point of focus in many investigations. In the present investigation, feasibility of metal atoms to form atomically thin metal flatland inside the graphene pore has been studied, the catalysis in such a modified frame has been examined.

Keywords: metal flatland; graphene pore; catalysis

P-067: Two - dimensional (2D) Oxides – Dichalcogenides - Carbides Heterostructures for Flexible Electronic Devices

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Abstract:

Extensive use of portable electronic products and the rapidly growing commercial markets in electric devices have created a seemingly high demand for flexible, wearable smart high-performance photoelectric devices and energy storage technology with higher energy and power densities. In the search for new materials to meet these criteria, one promising solution may be the 2D van der Waals heterostructures, assembled by stacking different conventional 2D materials (for example, graphene, transition metal oxides, carbides, and chalcogenides) in hetero-layered architectures. 2D van der Waals stackings are ultrathin layered crystals which show unusual physiochemical properties at few-atom thickness. In this work, we will develop various non-conventional growth techniques to fabricate 2D hetero-layers junctions of Graphene, hBN, TMOs, TMDs, MXene and then investigate the interfacial electronics. We will employ van der Waals epitaxy to stack different layers, and study the electronic properties, superlattice structure as well as the behaviour of electrical contact in the charge transport across the junction. The proposed work will focus on the fabrication method of transition metal Oxides and carbides and their possible heterostructures for the next generation 2D flexible optoelectronic and energy storage devices. The research outcomes will present a platform for an alternative way toward 2D-material-based electronics and van der Waals epitaxial growth by using an intermediate 2D oxide for energy storage devices.

Keywords: Two-dimensional materials; van der Waals Hetero-structures; Transition metal oxides; MXene; Energy Storage; flexible electronic devices

P-068: Nanocrystalline Electrochromic Tungsten Oxide Thin Films- Effect of Titanium Dopant

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Abstract:

In the present investigation, we have deposited titanium doped tungsten oxide thin films on to silicon wafer, quartz glass and indium doped tin oxide coated glass by using dc magnetron sputtering at different sputtering pressures and substrate temperatures. Emphasis being made on the effect of oxygen partial pressure and titanium doping on different characterizations. The films have good optical transmittance in the visible region of the spectrum and the optical band gap and refractive index of the films changes with deposition conditions. The structural properties of the films become amorphous due to doping with titanium at low substrate temperatures and it improves with the substrate temperature. The films contain both bending and stretching vibrations of O-W-O confirmed by micro Raman spectroscopy. The morphology of films varies between granular to coarse with the deposition conditions analysed from Field Emission Scanning Electron Microscopy and composition of the films contains both the elements of tungsten, oxygen and titanium given by Energy Dispersive Spectroscopy. The electrochromic properties like diffusion coefficients, switching speed and coloration efficiency of the films was evaluated from cyclicvoltammetry, chronoamperometry and chronocoulometry and the coloration efficiency of the films varied between 40.07 to 120.2 cm^2/C.

Keywords: WO_3; UV-VIS; XRD; FE-SEM and Electrochromism

P-069: Study of Positional Isomers for Spintronic Applications - A Theoretical Approach.

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Abstract:

Understanding the spin-dependent electron transport through a single molecular junction will provide in-depth knowledge to construct efficient molecular spintronic devices. The electron transport in such junction highly depends upon the structure of the molecule. Hence, we have studied the spin-dependent electron transport properties of positional isomers 4,6-dibromobenzene-1,3-dithiol; 2,4-dibromobenzene-1,3-dithiol and 2,5-dibromobenzene-1,3-dithiol using Density Functional Theory (DFT) with Non-Equilibrium Green's Function (NEGF). We have calculated the total density of states, projected density of states of the molecule, transmission spectra, current-voltage characteristic and magnetoresistance effect of these molecular junctions. The projected density of states of the molecule and the total density of states shows that these molecules have good coupling with the electrode. Under the applied bias, the spin up and spin down transmission varies in these molecular junctions which lead to magnetoresistance effect in these molecular junctions. Among these molecules, 2,5-dibromobenzene-1,3-thiol molecular junction shows a higher magnetoresistance effect than 4,6-dibromobenzene-1,3-dithiol and 2,4-dibromobenzene-1,3-dithiol. Hence, 2,5-dibromobenzene-1,3-thiol can be a good candidate for spintronic applications.

Keywords: Spintronics, molecular junction, positional isomers, Density Functional Theory, Non-Equilibrium Green’s Function.

P-070: Anisotropic Electron-Photon-Phonon Coupling in Layered MoS_2

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Abstract:

Transition metal dichalcogenide, especially MoS_2 has attracted lot of attention recently owing to its tunable visible range band gap and anisotropic electronic and transport properties. Here, we report a comprehensive inelastic light scattering measurements on CVD grown (horizontally and vertically aligned flakes) as well as single crystal flakes of MoS_2, probing the anisotropic optical response via studying the polarization dependence intensity of the Raman active phonon modes as a function of different incident photon energy and flake thickness. Our polarization dependent Raman studies intriguingly revealed strong anisotropic behavior reflected in the anomalous renormalization of the modes intensity as a function of flake thickness, phonons and photon energy. Our observations reflects the strong anisotropic light-matter interaction in this high crystalline symmetric layered MoS_2 system especially for the in-plane vibrations, which is crucial for understanding as well application of these materials for future application such as optoelectronic applications.

Keywords: 2D materials; Raman scattering; Electron-Photon–Phonon coupling

P-071: DFT study of the lead-free halide double perovskite and nitride materials for photovoltaics

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Abstract:

Organometal halide perovskites (OHP) and Nitrides are under intense study for use in optoelectronics. Among OHPs, the organometal lead halide perovskites have been emerged as the promising candidate as light harvesters in the solar cell with the first solar cell reported in 2009 [1] with improved photo-conversion efficiency now more than 22% [2]. A major element of flexibility in these materials is provided by creating halide mixtures to tune the bandgap over a range spanning the near-IR to near-UV wavelengths [3]. However, the toxicity of lead and moisture stability are two main obstacles with ABX3 for using it in commercial applications. An alternative possibility to replace Pb is proposed by heterovalent substitution by pairs of monovalent (B′ site) and trivalent cation (B″ site) to form double perovskite A2B′B″X6. The experimental and first-principles study of lead-free double perovskite have shown promising photovoltaic properties. However, some open problems are still prevailing the issue of double perovskite materials [4]. In present work, we explored the structural and elastic properties along with opto-electronic properties to assess the suitability of Double-perovskite and Nitride as flexible photovoltaic material. The elastic constants of the material provide information about the nature of forces acting in solid and consequently reflect structural stability, hardness, mechanical and dynamical behaviour of material. Our Calculations show that the electronic structure and optical properties of Double Perovskite halide and Sr-doped Nitride are suitable for photovoltaic applications.

Keywords: Photovoltaics, Density Functional Theory, Electronic structure

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P-072: First principle studies on Na_2LiAlH_6 for battery application

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Abstract:

For about a decade, the hydrides are considered as potential materials for the energy storage and conversion for battery application. The modern theory of Li-ion devices need high energy density and superior safety. The development of innovative electrode materials with excellent electrochemical performances is supposed to be the only way to satisfy the diversified and extended application of lithium-ion batteries (LIBs). Recently, the conversion materials, like metal hydrides are demonstrated as attractive, anode materials for LIBs due to their small polarization, high theoretical capacity and suitable working potential. Here, we report Na_2LiAlH_6 as a promising candidate for anode materials for Na-ion batteries. The calculation were performed utilizing density functional theory, implementing the generalized gradient approximation functional. Our calculation includes reaction mechanics of alkali metal, Density of states, Bader effective charge analysis to account the oxidation of the metal present in the system. Na_2LiAlH_6 is expected to be a promising candidate with high capacity and high rate capability for anode materials in Na-ion batteries. We hope that this work can stimulate more extensive and insightful studies for the fabrication and design of new metal hydrides with excellent physical and electrochemical performances.

Keywords: Anode Materials; Alkali-metal Hydrides; first Principle calculations; Na-ion batteries.

P-073: Title: Prediction of novel electronic phase due to breakdown of strong spin-orbit coupling in Iridates

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Abstract:

5d transition metal oxides, mainly Iridate where both electronic correlation and spin-orbit interaction are competing, forms a new play ground for emerging field of research with huge promise for realizing different novel phases of matter such as quenched magnetic phases, spin-orbit Mott insulator, topological phases etc. These various novel phenomena arise due to interplay of charge, lattice, orbital and spin degrees of freedom, which are governed by the "electrons". Therefore, understanding and prediction of such behavior from ab-initio perspective is indispensable aspect in this filed. This presentation is devoted to the prediction and investigation of microscopic origin of emerged counter-intuitive challenging quantum phase due to the breakdown of strong spin-orbit coupling in the Iridium based transition metal double perovskite Sr2CeIrO6, using density functional theory (DFT) based first principles electronic structure calculations. Our investigation challenges the common notion that for the half-filled Iridates, spin-orbit interaction is the most relevant energy scale and all the novel phenomena of iridates are driven by novel Jeff =1⁄2 states, realized via j-j coupling scheme. We revel that this simplistic common perception may not be the complete story of such systems. We predict that the delicate but crucial competition of different energy scales, viz. structural distortion, electronic correlation and spin-orbit interaction, drive counter-intuitive and unconventional anti-ferro orbital ordering even in the presence of spin-orbit interaction, which is beyond the framework of Jeff state perception. We also establish that the investigated material falls into unconventional class of intermediate coupling region between the two extremes, ideal L-S or j-j coupling.

P-074: First principles study on the dehydrogenation of ethylene diamine monoborane adducts and its cyclic products

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Abstract:

Dehydrogenation of Ethylene diamine mono borane (EDMB) adducts and its derivatives by substituting (R1/R2=H, CH_3, Cl, F, NH_2, OCH_3 and CN) have been performed to explore the potential candidate towards liquid organic hydrogen carrier (LOHC). Thermochemical properties such as energy, enthalpy and free energy change of these EDMB adducts and its dehydrogenated cyclic products (Monomer, Dimer and Trimer) were investigated. The free energy barrier calculation performed for the selected EDMB adducts such as 1. Cl/CN, 2. Cl/OCH_3, 3. F/CN, 4. F/OCH_3 5. F/F, 6. NH_2/H for cyclic monomer formation, 1. H/CH_3, 2. H/CN, 3. Cl/H, 4. NH_2/H for cyclic dimer formation and 1. H/Cl, 2. H/F, 3. NH_2/H for cyclic trimer formation shows promising candidate for chemical hydrogen storage. We also explored the cyclic trimer formation from the selected cyclic monomer such as 1. CH_3/CH_3, 2. H/CH_3, 3. NH_2/H. Reaction kinetics explains the dehydrogenation pathway through transition state calculation. Electrostatic surface potential and Frontier molecular orbitals also affirms the potential of the material through its electron redistribution and HOMO-LUMO gap regarding dehydrogenation kinetics.

Keywords: Ethylene diamine monoborane adducts; Thermochemistry; Liquid organic hydrogen carrier; Cyclic Products; Density Functional Theory

P-075: Near Infrared Spectroscopy as an efficient tool for the Qualitative and Quantitative Determination of Detergent Adulteraton in Milk

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Abstract:

Near Infrared Spectroscopy can act as a feasible tool for detecting the presence of detergent as an adulterant in milk. Present work was carried out to formulate a chemometric model to evaluate the presence of adulterating detergent in milk, qualitatively as well as quantitatively using NIR Spectroscopy. Total 30 samples were prepared using three different varieties of milk, out of which three samples was free from adulterants and rest were having detergent present in them. Those 27 milk samples were adulterated with detergent at nine different levels: 0.025%, 0.05%, 0.1%, 0.2%, 0.4%, 0.6%, 0.8%, 1.0% and 2.0% of detergent respectively for each kind of milk. The data collected from NIRS instrument was analyzed using chemometric software (CAMO Unscrambler version X 10.3). The Principal Component Analysis (PCA) was run on the sample set to know the relation between the different samples on the basis of the Near Infrared spectral data. It was noticed that the PCA score plot could classify the samples in three groups on the basis of their adulteration: low, medium and high adulteration. Partial least square regression analysis (PLS-RA) was used to develop a statistical model to predict the percentage of detergent present in the adulterated milk samples by selecting vital wavelengths. It was analysed that the regression model revealed quite good results for the prediction of detergent adulterated milk samples with coefficient of correlation higher than 0.9 and the root means square error of validation (RMSEV) was 0.013. Thus, it was agglomerated that NIR spectroscopy could provide dairy industry a simple, efficient, quick, green and non-destructive technique for detection and quantification of milk adulteration.

Keywords: Milk; Adulteration; Near Infrared Spectroscopy; Regression; Chemometrics.

P-076: Investigations on Highly photocatalytic CTAB templated Titania nanoparticles doped with Europium

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Abstract:

Europium-doped cetyltrimethylammonium bromide (CTAB) surfactant assisted Titania nanoparticles were prepared by a solvothermal method with ethanol as solvent. The prepared nanoparticles were examined using various characterization techniques such as X-ray diffraction (XRD), Fourier transform infrared microscopy (FTIR), Transmission electron microscopy (TEM), high-resolution electron microscopy (HRTEM), Energy dispersive spectrum (EDS) and Ultraviolet – diffuse reflectance microscopy(UV -DRS). XRD patterns exhibit the anatase phase of titania with highly crystalline nature. Crystallite sizes calculated from XRD peaks range between 4 to 10nm.TEM and HRTEM analysis reveals the particle size and morphology of the prepared samples. Photocatalytic measurements for the samples were carried out and they exhibit high efficiency of photodegradation.

Keywords: surfactant; titania; solvothermal; photocatalytic

P-077: Investigation on growth and optical characterization of L-Alanine Potassium Hydrogen Orthophosphate Single crystal for laser application

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Abstract:

A new semi-organic nonlinear optical crystal called L-Cysteine Di-Potassium Hydrogen Orthophosphate was synthesized. The single crystal was grown from an aqueous solution using the Slow Evaporation Method. Crystal have been grown with a solution. Single crystal X-ray Diffraction (XRD) study was carried-out to identify the lattice parameters. Various diffracting planes of the grown crystal were identified from the powder XRD study. The FT-IR spectroscopic technique was used to find out the various characteristic absorption bands & functional groups present in the grown crystal. The transmission spectrum of this crystal shows that the lower cut off wavelength lies at 260 nm. The thermal stability and decomposition pattern of the compound were formulated using TGA-DTA studies. The UV-Visible absorption study was studied to ascertain the optical property of the compound. The heating and cooling cycles observed in differential thermal analysis (DSC) indicates that the grown crystal shows first order phase transition.

P-078: Hydrogen storage in Ti-decorated porous graphene

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Abstract:

The H_2 adsorption on pure and Ti-decorated porous graphene has been studied using Density Functional Theory (DFT). The computations have been done using DFT based DMol^3 code. The exchange and correlation functional has been approximated by the simplest and efficient Density Functional Approximation (DFA), Local Density Approximations (LDA). The convergence tolerance corresponding to energy, maximum force and maximum displacement has been set to 1.0×10^{-4} Ha, 0.02 Ha/Å and 0.05 Å respectively for geometry optimization. To increase the interaction binding energy and storage capacity, the surface of porous graphene has been decorated by Ti atoms. After the decoration, the adsorption binding energy of H_2 is enhanced. Up to five H_2 molecules adsorb molecularly on each Ti atom anchored on PG and this leads to the configuration PG-8(Ti+5H_2) with a gravimetric capacity of 7.58 wt%. Molecular dynamics simulation at 300 K shows that the H_2 molecules are stably adsorbed around Ti atom. The Partial Density Of States (PDOS) projected to PG shows that there is a nonzero state at the Fermi energy and so the system is metallic. The presence of sharp peaks at -5 eV corresponding to d states of Ti atoms in the middle panel and the s states that belongs to the H_2 molecule in the lower panel shows that hybridization occurs between these states. This interaction is also widely known as the Kubas interaction. This interaction involves hybridization between the partially filled and partially empty 3d orbitals of the transition metal atom and the σ (both bonding and anti- bonding) orbitals of H_2.

Keywords: nanomaterials; density functional theory; graphene

P-079: Extracellular Matrix from Marine Invertebrates for Faster Biomineralization and tailored mechanical properties of scaffolds with tunable interconnected porous architecture for bone regeneration

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Abstract:

The extraction and purification of collagen are of great interest due to its biological function and medicinal applications. Although marine invertebrates are abundant in the animal kingdom, our knowledge of their extracellular matrix (ECM), which mainly contains collagen, is lacking. The functions of collagen isolated from marine invertebrates remain an untouched source of the proteinaceous component in the development of groundbreaking pharmaceuticals. Although hydroxyapatite (HA) based porous scaffolds are being widely researched in last three decades, the development of naturally-derived biomimetic with tunable elastic modulus and strength together with faster biomineralization property has not yet been achieved. The improved proliferation of bone mesenchymal stem cells (BMSCs) when they are induced with TCP-Mg, glucose consumption and ALP activity was observed for 1–2.5 mm TCP-Mg compared with granules of pore size ($P < 0.05$). In addition, BMSCs incubated with 1–2.5 mm TCP-Mg expressed significantly higher levels of the genes for a runt-related transcription factor. The osteogenesis-related proteins compared with BMSCs incubated with TCP-Mg ($P < 0.05$). Fluorochrome labeling and histological staining analyses indicated that the osteo-regenerator with two holes perforating significantly greater bone regeneration compared with the other osteo-materials. To address this specific issue, we report here a scalable biogenic synthesis approach to obtain submicron TCP powders from Sea Urchin Spines. The marine resource derived TCP together with different pore formers can be conventionally sintered to produce scaffolds physiologically relevant with porous architecture.

Keywords: collagen; corals; Osteogenesis; scaffold; biomineralization; Seaurchin; porosity

P-080: Structural, Optical and Luminescence properties of Core Shell heterostructure $CdSZn_3(PO_4)_2$ Nanocomposite for LED application

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Abstract:

Inorganic semiconducting $CdSZn_3(PO_4)_2$ nanocomposite synthesized at mild reaction temperature of 100°C under hydrothermal method. The prepared nanocomposite is investigated by Powder X-ray diffraction, UV-Vis absorption, Diffusion Reflectance spectra, FT-IR spectra, Scanning electron microscope, and Photoluminescence techniques in a systematic manner. XRD shows peaks corresponding to hexagonal structure of CdS and monoclinic γ-phase of $Zn_3(PO_4)_2$ with good crystalline nature.. Interstingly, due to coupling of CdS with $Zn_3(PO_4)_2$ it shows the phase transition from α-Phase of $Zn_3(PO_4)_2$ to γ-phase of $Zn_3(PO_4)_2$ under hydrothermal conditions and also there is internal structural variations due to the formation of $CdSZn_3(PO_4)_2$ nanocomposite. Average crystallite size, lattice strain and dislocation density are estimated by Debye-Scherrer and W-H method. The average crystal lattice is found to be 15-25nm. The surface morphology of prepared composite shows the hexagonal spheres accumulated on rectangular flakes which indicate core-shell heterostructure. From UV–Vis absorption spectra, the absorption wavelength exist in the visible region due quantum size effects and energy band gap is 2.42eV. FT-IR spectrum shows the fundamental vibrational modes of $CdS/Zn_3(PO_4)_2$. The photoluminescence spectrum exhibits broad intense luminescence band in visible region of wavelength 510-518nm range which is in good agreement with absorption wavelength and from CIE diagram, Colour coordinate values and CCT values of the prepared composites are utilized for LED applications.

Keywords: CdS; $Zn_3(PO_4)_2$; Nanocomposite

P-081: Magnetoelectric properties of self-assembled close-packed free-standing $CoFe_2O_3$ - $Pb(Zr,Ti)O_3$ thin films

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Abstract:

Multiferroic composite thin film with promising larger magnetoelectric (ME) effects become a recent scenario of ever-increasing interest in last few decades due to their multifunctionality.[1,2] This material has the potential to lead the development of a multifunctional device like ME random access memories,[3] ME microsensor[4]. We report on the fabrication of a free-standing multiferroic thin film [$(Co_{0.95}Fe_{2.05}O_4)$CFO/ $(Pb(Zr_{0.52}Ti_{0.48})O_3)$PZT] with close-packed structure has been prepared by the combination of self-assembly and RF sputtering technique and its magnetoelectric (ME) characteristics have been evaluated and compared with the planar multiferroic composite thin film. The hollow space inside the free-standing structure which could alleviate the clamping force at the interface of CFO/PZT to enhance the superimposition of the ferromagnetic and ferroelectric phases in the free-standing multiferroic thin film. Our goal of the present study is the enhancement of strain mediated ME coupling mechanism by deteriorating the substrate clamping force in the free-standing CFO/PZT multiferroic thin film. While comparing the free-standing structure with the planar film, the constraint by the substrate is alleviated by the hollow space inside the shell. It is expected that a large ME effect will be developed.

Keywords: Multiferroic; RF Sputtering; free- standing.

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P-082: First principle study of Adsorption Behavior of PF_5 gas molecule on S and Mo vacancy MoS_2 Monolayer

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Abstract:

Molybdenum disulfide monolayer (MoS_2) gains more attention due to its attractive electronic property and it is widely used in different electronic applications. The presence of vacancy on MoS_2 monolayer leads to increase in conductivity of the material. In this work we have investigated the adsorption behavior and estimate the gas sensing properties of S and Mo vacancy MoS_2 monolayer with PF_5 gas molecules. To explore the sensing and electronic property of PF_5 gas molecule the geometrical structures, adsorption distance, adsorption energy, charge transfer, band structure and density of the states were analyzed. The results show that the PF_5 gas molecule is allowed to adsorb on S and Mo vacancy MoS_2 monolayer through Van Der Waals interaction. PF_5 gas molecule exhibits the adsorption distance of 3.3274Å, 2.8673 Å adsorption energy of-0.1640eV,0.3489 eV and charge transfer of 0.025 Q(e), 0.053 Q(e) on S and Mo vacancy MoS_2 monolayer. The results predicted that the Mo vacancy MoS_2 monolayer shows relatively more adsorption towards PF5 gas molecule.

Keywords: Density Functional Theory(DFT); Band Structure; Density of the States.

P-0F1: Modeling Fracture in Porous Rock

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Abstract:

Most of the rocks and soil are porous and can carry water and other fluids like oil and natural gases. To have a better understanding of how these fluids ow or how to recover them (in oil and gas industry) it is necessary to model and characterize the porous media and fracture in it properly. Here a Porous rock is generated by depositing spherical elements with random size under gravity using Discrete Element Method (DEM)1. We have studied the porosity, pore distribution and pore connectivity of the generated sample for different size distributions of the spherical elements. Fractal nature of the pore has been investigated through diffusion studies. Fracture has been generated by applying compressional stress on the porous media. Translational and rotational displacement of the spherical grains is allowed under stress. The cementing material joining the grains fractures when a threshold stress is exceeded. The change in the micro geometry of the fractured structure is studied with respect to varying fracture threshold.

Keywords: Porous Media; Fracture; DEM; Fractal

P-0F2: Variation from frosted to glassy texture and change in fractal character of desiccation cracks on acidifying a clay suspension

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Abstract:

Laponite particles possess anisotropic nanometric shape having dissimilar charge distributions. It is a synthetic clay material, is known to have wide spread applications as a rheology modifier and as reinforcement in variety of industries. Aqueous laponite dispersion shows a rich variety of phase behaviors that share complex interactions. We have shown that the change of the pH of the aqueous laponite dispersion shows different phase behaviors depending on the pH of the suspension. It shows a glass transition at a certain pH range having low conductivity of the dispersion. Analysis of the rheological response leads to fractal, which is actually seen in case of low pH and for high pH, it changes to different phase which forms cracks. The conductivity of the suspensions, which depends on the pH of the suspension, plays an important role during formation of cracks. Characterization of the fractals and cracks shows different type of properties. An important behavior is seen at high pH and concentration i.e. a lace like behavior is observed at a fixed drying condition. We are trying to analyze the lace like patterns observing the SEM image and EDAX.

P-0F3: Response of Glassy Liquids to Thermal Gradients

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Abstract:

The response of a model glass-forming liquid [1] to an externally applied thermal gradient has been studied using extensive non-equilibrium molecular dynamics simulations [2][3]. In the supercooled liquid regime, we have demonstrated that the mixture responds by the formation of concentration gradients, which are dependent on the local temperature. The interplay between the transport processes, related to temperature and concentration, occurring in the system, is characterized via the Soret-coeffcient, which is the ratio of the thermal diffusion coeffcient and inter-diffusion coeffcient. The behavior of Soret-coeffcient in supercooled regime is found to increase as the temperature is lowered, which we relate to the behaviour of the inter-diffusion coeffcient near the mode-coupling temperature. In the supercooled regime, we also observed that when larger thermal gradients are imposed, the spatial profiles of the particle concentrations become non-linear. We have characterized in details how the onset of the non-linear regime depends on the mean temperature and the thermal gradient. The response near glassy regime has also been explored: local concentration is almost not affected, in the presence of the thermal gradient, wherever local
temperature is below mode-coupling temperature.

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P-0F4: Cavitation transition in pinned glass-forming liquids

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Abstract:

When a glass forming liquid is expanded across the binodal line in the phase diagram, it undergoes an abrupt failure via cavitation. In our numerical simulations, we study how in the athermal quasistatic limit, this undesirable and abrupt cavitation process can be altered to a qualitatively different and gradual transition by pinning a small fraction of particles. The presence of pinned sites, localises the relaxation, leading to formation of multiple cavities in the system as observed via spatio-temporal probes on the system.

P-0F5: Crack growth in heterogeneous environment

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Abstract:

Crack growth in brittle materials is addressed in general within the framework of continuum mechanics which relates deterministically the applied stress to the length of the crack to make the crack unstable. However, in heterogeneous materials, the crack dynamics is much more complicated involving intermittency and crackling. We study the crack growth in the so-called nominally brittle materials by inserting and studying the growth of a dominant crack in a model heterogeneous system namely the fibre bundle model. We find that the disorder or heterogeneity in the model introduces a characteristic length scale ξ directly proportional to the strength of the disorder. If the length l of the pre-existing crack is less than ξ, the presence of the crack does not influence the crack growth and fracture. Loading, in this regime, causes spalling of the material through the nucleation, growth and coalescence of multiple cracks exhibiting avalanches. On the other hand, when $l > \xi$, the rupture occurs due to the extension of the pre-assigned dominant crack. In this regime, the critical strength at the depinning of the crack varies as $l^-{\alpha}$. $\alpha ~ 0.84$ for strong disorder.

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