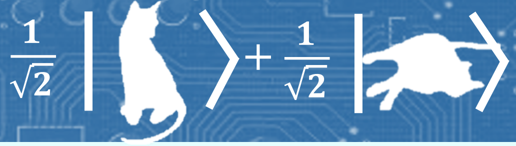
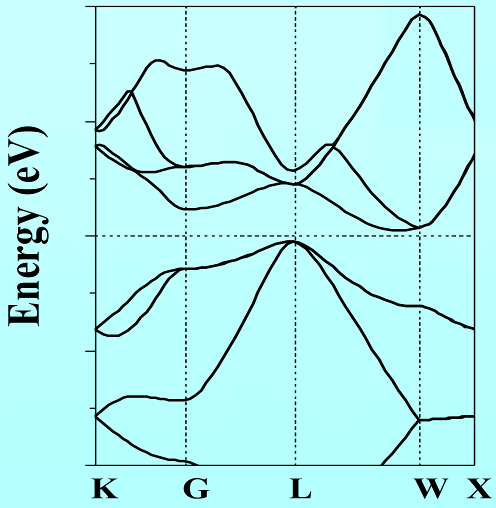
$$H\psi_n(\rho(r)) = \varepsilon_n \psi_n(\rho(r))$$

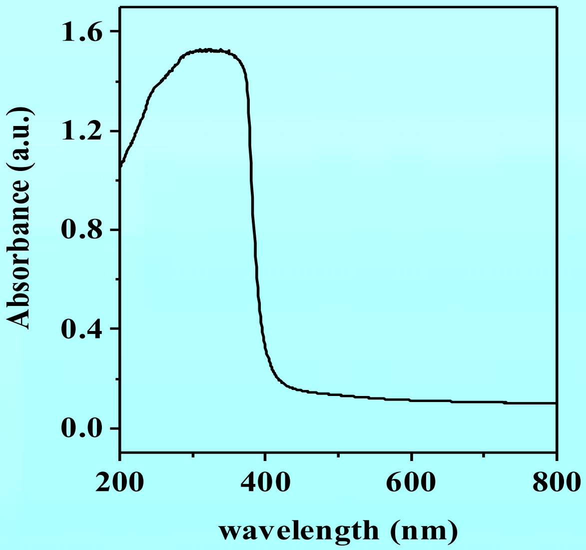


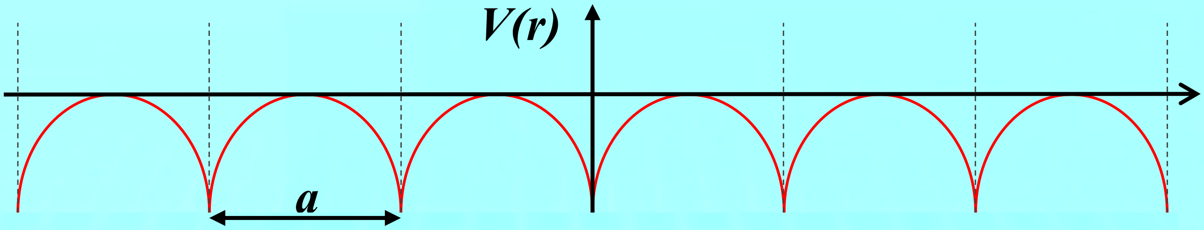
INTERNATIONAL WORKSHOP AND CONFERENCE ON **EVOLUTION OF ELECTRONIC STRUCTURE THEORY & EXPERIMENTAL REALIZATION**

(EESTER-2020)

14 – 18th December 2020 in online mode







SRM
INSTITUTE OF SCIENCE & TECHNOLOGY
(Deemed to be University u/s 3 of UGC Act, 1956)

Jointly organized by

SRM INSTITUTE OF SCIENCE AND TECHNOLOGY, KTR, INDIA
INDIAN INSTITUTE OF TECHNOLOGY MADRAS, INDIA
UPPSALA UNIVERSITY, SWEDEN

International Workshop and Conference on

Evolution of Electronic Structure Theory and Experimental Realization

(EESTER 2020) 14th -18th December, 2020 in webinar mode

Organizers: SRMIST KTR (India), IIT Madras (India) and Uppsala University (Sweden)

Visit us: https://www.srmist.edu.in/eester-2020/: Contact Us: eester.2020@srmist.edu.in

Dear Speakers and Participants,

It is a great pleasure to welcome you all to the second edition of the international conference and workshop on the Evolution of Electronic Structure Theory and Experimental Realization (EESTER). The success of the first edition in 2018, encouraged us to organize it a second time, albeit in a webinar mode, during this pandemic period.

In this edition, we will have 26 invited talks, 12 oral presentations, and 32 poster presentations. We have categorized the invited talks in three groups - plenary lectures (colloquium style) aiming at providing the broader picture of a certain topic, workshop lectures to impart basic insights of the methods, and research lectures to discuss recent progress in the area of electronic structure in specific and condensed matter physics in general. Due to time constraint, attempts are made to give scope to the senior graduate students and post-doctoral fellows to make oral presentations while the other enthusiasts are accommodated through poster presentations.

We have made a thematic based gelling of experimental, computational and theoretical talks, as electronic structure calculations and experimental studies go hand-in-hand, hoping that students will be benefitted the most.

We highly appreciate the speakers for their ready acceptance of our invitation. We are confident that the conference will result in tremendous learning for each one of us including the research scholars and post-doctoral fellows from various universities and institutes from India and abroad.

We are looking forward to a great conference. Your active participation and support will make EESTER 2020 a greater success than EESTER 2018 and will help us to crystallize this event as a biennial event.

Best regards,

Organizers EESTER 2020

Biplab Sanyal

Saurabh Ghosh

Jaivardhan Sinha

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It is my great pleasure to be a part of the organization of EESTER, 2020. I believe that this type of scientific event is very important to bring theoreticians and experimentalists together in the field of materials science for a meaningful development of knowledge for the young scientists, in particular. Due to the current pandemic situation, we had to organize it online but the enthusiasm in the participation is very encouraging for us to realize that scientific practice will find its own way in any difficult situation. I wish that all the participants will have a wonderful and fruitful experience for the entire week.

Best regards,

Biplab Sanyal

Biplab Sanyal
Ph.D., Docent
Associate Professor & Division Head
Division of Materials Theory,
Dept. of Physics and Astronomy,
Uppsala University, Sweden

INDIAN INSTITUTE OF TECHNOLOGY MADRAS
Chennai 600 036 (INDIA)

Ashok Kumar Mishra
Dean Academic Research

13 December, 2020

I am pleased to learn that IIT Madras, SRMIST and Uppsala University have come together to organize the second edition of the EESTER-2020. With the formulations of state-of-the art many-body techniques and aided with AI as well as machine learning, the electronic structure theory has come closer than ever before to explain the experimental observations and pave way for design of new materials. The present edition of EESTER is contextual and a timely event. This conference-cum-workshop offers the participants basic insights on methods and formalisms. Besides, it adequately covers recent progresses in condensed matter physics and materials science too. I am certain that every attendee will gain significantly from this event.

I welcome you all and wish the event a great success.

- Ashok Mishra

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(Deemed to be University u/s 3 of UGC Act, 1956)

Prof. K. Ramasamy
Director (Research),
SRM Institute of Science and Technology, KTR, Tamil Nadu, India

We welcome the participants and the speakers to the online International Conference and Workshop on *Evolution of Electronic Structure Theory and Experimental Realization (EESTER-2020)* jointly organized by SRMIST, IIT Madras and Uppsala University, Sweden.

The main objective of this joint program is to introduce various methods for electronic structure calculations, discuss the present theoretical progresses concerning to many-body theory and how experiments are driving and contributing to such progresses. The other important purpose of this joint program is to impart fundamental understanding to the graduate students and post-docs pursuing their research in electronic structure. In the days of pandemic, it is difficult to meet you and interact, but virtual zoom helps us to progress in research capacity.

I hope this Conference and Workshop would greatly benefit young research scholars in the related field and I wish all success for the efforts put together by SRMIST, IIT Madras and Uppsala University, Sweden.

Such multi institutional participatory system should deliver inter disciplinary contribution towards knowledge, product, and creativity leading to societal development.

Wish you all the success.

K. Ramasamy

December 11, 2020

International Workshop and Conference on

Evolution of Electronic Structure Theory and Experimental Realization (EESTER 2020)

Jointly Organized by SRM IST KTR (India), IIT Madras (India) and Uppsala University (Sweden)

December 14- 18, 2020 in online mode

Inaugural Session: Day 1, 14th December 2020, Monday

8:30 am - 9:00 am (Central European Time) / 1:00 pm - 1:30 pm (Indian Standard Time)

Program Schedule	**Day 1**	**Day 2**	**Day 3**	**Day 4**	**Day 5**
	14th December Monday	15th December Tuesday	16th December Wednesday	17th December Thursday	18th. December Friday

PL = Plenary Lecture
(45 minutes talk + 15 minutes discussion)
WL = Workshop Lecture
(45 minutes talk + 15 minutes discussion)
SL = Seminar Lectures
(30 minutes talk + 10 minutes discussion)
CET = Central European Time

OP = Oral Presentations
(12 minutes talk + 3 minutes discussion)
PO= POSTER Presentations
(3 minutes pre-recorded YouTube Video link
+ 2 minutes Q&A)

IST = Indian Standard Time

Demonstration of Electronic Structure code Quantum Espresso

- Day 4: 10:00 am – 12:30 pm (IST) for participants login from India
- Day 4: 3:00 pm - 5:30 pm (CET) for participants login from Europe/US/Brazil

Day 1: 14th December, Session 1, 9:00 am – 12:00 pm CET / 1:30 pm – 4:30 pm IST

PL1: Theory

CET 9:00 am – 10:00 am
IST 1:30 pm – 2:30 pm

Prof. G. Baskaran, IIT Madras, India, IMSc, Chennai, India & Perimeter Institute, Waterloo, Canada

Theory of Electronic Structures from Experimental Results - The Anderson Way

PL2: Theory

CET 10:00 am – 11:00 am
IST 2:30 pm – 3:30 pm

Prof. Olle Eriksson, Uppsala University, Sweden

DFT and fundamentals of electronic structure calculations

PL3: Experiment

CET 11:00 am – 12:00 pm
IST 3:30 pm – 4:30 pm

Prof. D. D. Sarma, Indian Institute of Science Bangalore, Bengaluru, India

An introduction to photoelectron spectroscopy: How to estimate electronic parameter strengths from experiments

Break 20 Minutes : 12:00 pm – 12:20 pm (CET) / 4:30 pm - 4:50 pm (IST)

Day 1: 14th December, Session 2, 12:20 pm – 3:30 pm CET / 4:50 pm – 8:00 pm IST

POSTER (PO)

CET 12:20 pm -12:40 pm
IST 4:50 pm – 5:10 pm

POSTER Theory Application (PTA)-1, 2, 3, 4

SL1: Theory CET 12:40 pm – 1:20 pm IST 5:10 pm – 5:50 pm	 **Prof. Hena Das,** Tokyo Institute of Technology, Yokohama, Japan *Microscopic origin of near room-temperature multiferroic phenomena in* $(LuFeO_3)_m/(LuFe_2O_4)_1$ *superlattices*
SL2: Experiment CET 1:20 pm -2:00 pm IST 5:50 pm -6:30 pm	 **Prof. A. Sundaresan,** JNCASR, Bangalore, India *Multiferroic Properties and Unconventional Spin Density Wave in Doubly Ordered Perovskite* $NaLnNiWO_6$ *(Ln=Y, Dy, Ho, and Yb)*
SL3: Theory CET 2:00 pm – 2:40 pm IST 6:30 pm - 7:10 pm	 **Prof. Biswarup Pathak,** Indian Institute of Technology Indore, India *Nano-electrodes for ultrafast DNA sequencing*
POSTER (PO) CET 2:40 pm - 3:00 pm IST 7:10 pm – 7:30 pm	**POSTER Theory Application (PTA)- 5,6,7,8**
POSTER (PO) CET 3:00 pm – 3.30 pm IST 7:30 pm - 8:00 pm	**Open Forum Discussion on POSTER presentations**

Day 2: 15th December, Session 1, 9:00 am – 12:00 pm CET / 1:30 pm – 4:30 pm IST

WL1: Theory CET 9:00 am – 10:00 am IST 1:30 pm – 2:30 pm	 **Prof. G.P. Das,** Indian Institute of Technology Kharagpur, India *DFT in condensed systems : some practical guidelines*
WL2: Theory CET 10:00 am – 11:00 am IST 2:30 pm – 3:30 pm	 **Prof. Aftab Alam,** Indian Institute of Technology Bombay, Mumbai, India *Broken symmetry driven topological semi-metal to gaped phase transition in SrAgAs*
WL3: Theory CET 11:00 am – 12:00 pm IST 3:30 pm – 4:30 pm	 **Prof. Indra Dasgupta,** Indian Association for the Cultivation of Science, Kolkata, India *Modeling Strongly Correlated Systems*

Break 20 Minutes : 12:00 pm – 12:20 pm (CET) / 4:30 pm - 4:50 pm (IST)

Day 2: 15th December, Session 2, 12:20 pm – 3:30 pm CET / 4:50 pm – 8:00 pm IST

POSTER (PO) CET 12:20 pm -12:40 pm IST 4:50 pm – 5:10 pm	**POSTER Theory Application (PTA)- 9,10,11,12**
SL4: Theory CET 12:40 pm – 1:20 pm IST 5:10 pm – 5:50 pm	 **Prof. Alessandro Stroppa,** CNR-SPIN, Italy *Electric dipole ordering and spin-orbit interaction in hybrid organic-inorganic perovskites*
SL5: Theory CET 1:20 pm -2:00 pm IST 5:50 pm -6:30 pm	 **Prof. Tanmoy Das,** Indian Institute of Science Bangalore, India *Topological phases of matter*
PL4: Theory CET 2:00 pm -3.00 pm IST 6:30 pm - 7:30 pm	 **Prof. Sokrates Pantelides** Vanderbilt University, Nashville, USA *Adventures and discoveries in layered two-dimensional ferroelectrics*
POSTER (PO) CET 3:00 pm – 3.30 pm IST 7:30 pm - 8:00 pm	**POSTER Theory Application (PTA)- 13,14,15,16,17, 18**
Day 3: 16th December, Session 1, 9:00 am – 12:00 pm CET / 1:30 pm – 4:30 pm IST	
PL5: Machine Learning CET 9:00 am – 10:00 am IST 1:30 pm – 2:30 pm	 **Prof. Tamio Oguchi,** Osaka University, Japan *Machine Learning Applied to Materials Science*
Oral Presentations (OP) CET 10:00 am – 11:00 am IST 2:30 pm – 3:30 pm **OTD= ORAL Theory Development**	**OTD-1: Bikash Patra**, National Institute of Science Education and Research, Bhubaneswar, India *Relevance of the Pauli kinetic energy density for semilocal functional* **OTD-2: Dr. Igor Di Marco,** Asia Pacific Center for Theoretical Physics, South Korea *Determining the Intra-Atomic Exchange Energy in Rare-Earth Adatoms* **OTD-3: Aditi Mandal,** Birla Institute of Technology and Science, Pilani, India *Brief description of Plasmon excitation within multiple scattering approach Photoemission energy loss spectroscopy* **OTD-4: Dr. Subhayan Roychoudhury**, Lawrence Berkeley National Laboratory, USA *Neutral excitation density functional theory: a variational first-principles method for simulating excitations in molecules*

<table>
<tr><td>**Oral Presentations (OP)**
CET 11:00 am – 12:00 pm
IST 3:30 pm – 4:30 pm

OTA= ORAL Theory Application</td><td>**OTA-1: Santanu Pathak**, Variable Energy Cyclotron Centre, Kolkata,India
Precision measurement and electronic structure calculations for understanding the microscopic and macroscopic properties of HfO_2

OTA-2: Namrata Jaykhedkar, Faculty of Natural Sciences, Slovakia
Theoretical study of temperature dependent behaviour of crystal phase in $SrZrS_3$

OTA-3: Shashi Bhusan Mishra, IIT Madras, Chennai, India
Formation of a suspended magnetic layer between graphene layers through fluorine intercalation

OTA-4: Dr. Tisita Das, Harish-Chandra Research Institute, Allahabad, India
Enhanced Hydrogen Evolution Activity at the Edges of $MPSe_3$ *(M=Mn, Fe) Tri-chalcogenide Layers*</td></tr>
<tr><td colspan="2">**Break 20 Minutes : 12:00 pm – 12:20 pm** (**CET**) **/ 4:30 pm - 4:50 pm (IST)**</td></tr>
<tr><td colspan="2">**Day 3: 16th December, Session 2, 12:20 pm – 3:30 pm CET / 4:50 pm – 8:00 pm IST**</td></tr>
<tr><td>**POSTER (PO)**
CET 12:20 pm -12:40 pm
IST 4:50 pm – 5:10 pm</td><td>**POSTER Theory Development (PTD)-1,2**

POSTER Theory Application (PTA)- 19, 20</td></tr>
<tr><td>**SL6: Machine Learning**

CET 12:40 pm – 1:20 pm
IST 5:10 pm – 5:50 pm</td><td>
Prof. Ranjit Thapa SRM University-AP, Amravati, India

Descriptor to define the activity of carbon catalyst for OER: Quantum Mechanics and Machine Learning Approach</td></tr>
<tr><td>**SL7: Machine Learning**

CET 1:20 pm -2:00 pm
IST 5:50 pm -6:30 pm</td><td>
Prof. Tarak Patra Indian Institute of Technology Madras, Chennai, India

Deep Learning and Active Learning of Interatomic Force Fields</td></tr>
<tr><td>**PL6: Machine Learning**

CET 2:00 pm – 3.00 pm
IST 6:30 pm - 7:30 pm</td><td>
Prof. Rampi Ramprasad, Georgia Tech, USA

Polymer Informatics: Current Status & Critical Next Steps</td></tr>
<tr><td>**POSTER (PO)**

CET 3:00 pm – 3.30 pm
IST 7:30 pm - 8:00 pm</td><td>**POSTER Theory Application (PTA)- 21, 22, 23, 24, 25**</td></tr>
<tr><td colspan="2"></td></tr>
<tr><td colspan="2">**Day 4: 17th December, Session 1, 9:00 am – 12:00 pm CET / 1:30 pm – 4:30 pm IST**</td></tr>
<tr><td>**PL7: Experiment**

CET 9:00 am – 10:00 am
IST 1:30 pm – 2:30 pm</td><td>
Prof. Joachim Mayer, RWTH Aachen University, Germany

Atomic Scale Imaging and Spectroscopy with Aberration Corrected Transmission Electron Microscopy</td></tr>
</table>

WL4: Experiment CET 10:00 am – 11:00 am IST 2:30 pm – 3:30 pm	 **Prof. Kalobaran Maity,** Tata Institute of Fundamental Research, Mumbai, India *Spectroscopy for electronic structure analysis*
WL5: Experiment CET 11:00 am – 12:00 pm IST 3:30 pm – 4:30 pm	 **Prof. Bent Weber,** Nanyang Technological University, Singapore *Proximity-Induced Superconductivity in Epitaxial Quantum Spin Hall Heterostructures*
Break 20 Minutes : 12:00 pm – 12:20 pm (**CET**) **/ 4:30 pm - 4:50 pm (IST)**	
Day 4: 17th December, Session 2, 12:20 pm – 3:30 pm CET / 4:50 pm – 8:00 pm IST	
CET 12:20 pm -12:40 pm IST 4:50 pm – 5:10 pm	**Open Forum for Discussion on Demonstration of Quantum Expresso**
SL8: Experiment CET 12:40 pm – 1:20 pm IST 5:10 pm – 5:50 pm	 **Prof. Srimanta Middey,** Indian Institute of Science, Bangalore, India *Defect induced emergent phenomena at the surface and interface of band insulators*
SL9: Experiment CET 1:20 pm -2:00 pm IST 5:50 pm -6:30 pm	 **Prof. Ravi Singh,** IISER Bhopal, India *Role of Disorder, Spin Orbit Coupling and Magnetism in the Electronic Structure of Ir Based Double Perovskite*
PL8: Theory CET 2:00 pm – 3.00 pm IST 6:30 pm - 7:30 pm	 **Prof. Lars Nordstrom,** Uppsala University, Sweden Complex magnetic order and their spontaneous spin and charge currents
CET 3:00 pm – 3.30 pm IST 7:30 pm - 8:00 pm	Demonstration: Quantum Espresso for participants login from outside India contd.

Day 5: 18th December, Session 1, 9:00 am – 12:00 pm CET / 1:30 pm – 4:30 pm IST	
PL9: Theory CET 9:00 am – 10:00 am IST 1:30 pm – 2:30 pm	 **Prof. Annica Black-Schaffer,** Uppsala University, Sweden *Topological superconductivity and Majorana fermions*

WL6: Machine Learning CET 10:00 am – 11:00 am IST 2:30 pm – 3:30 pm	 **Prof. Abhishek Singh,** Indian Institute of Science Bangalore, India *Machine learning and its application in Materials Science: Role of various Algorithms*
WL7: Experiment CET 11:00 am – 12:00 pm IST 3:30 pm – 4:30 pm	 **Prof. Avinash V. Mahajan,** Indian Institute of Technology Bombay, India *Novel states in magnetism: low-dimensional systems and spin liquids*

Break 20 Minutes : 12:00 pm – 12:20 pm (CET) / 4:30 pm. - 4:50 pm (IST)

Day 5: 18th December, Session 2, 12:20 pm – 3:20 pm CET / 4:50 pm – 7:50 pm IST

ORAL Presentations CET 12:20 pm – 1:20 pm IST 4:50 pm – 5:50 pm Oral Presentations Experiment (OEX)	**OEX-1: Abhishek Maiti**, Indian Association for the cultivation of Science, Kolkata, India *Rashia Band Splitting in Methylammonium Lead Iodide: An Insight from Spin-Polarized Scanning Tunnelling Spectroscopy* **OEX-2: Sameer Kumar Mallik,** Institute of Physics, Bhubaneswar, India *Hysteresis study in salt-assisted CVD grown monolayer MoS2 field-effect transistor by pulsed I~V technique* **OEX-3: Dr. Rajib Batabyal,** Niels Bohr Institute, Denmark *Topological Fermi-arcs and Weyl node connectivity in ferromagnetic Weyl semimetal* $Co_3Sn_2S_2$ **OEX-4: Dr. Sofi Suhail Majid,** Institute of Physics, Taiwan *Unveiling the role of V-V dimerization on insulator-metal transition and optical transmittance of* VO_2 *thin films*
Oral Presentations CET 1:20 pm – 1:45 pm IST 5:50 pm – 6:15 pm	**POSTER Experiment (OEX)-1,2,3,4,5**
CET 1:45 pm – 2:05 pm IST 6:15 pm – 6:35 pm	**Open slot for discussion / reschedule talk**
SL10: Experiment CET 2:00 pm – 2.40 pm IST 6:35 pm - 7:15 pm	 **Prof Shibayan Roy** Indian Institute of Technology Kharagpur, Kharagpur, India *Atomic scale experimental characterization complimented by atomic scale simulations for component scale materials designing*
Concluding Session CET 2:45 pm – 3.15 pm IST 7:15 pm – 7:45 pm	**Prize Distribution, Feedback from Participants & Vote of Thanks** Biplab Sanyal, Ranjit Nanda, Sudakar Chandran, Saurabh Ghosh, Jaivardhan Sinha and other invited guests 

EESTER 2020 ORAL Presentations

SL. No	Name & Affiliation	Title	Category	Presentation Number	Schedule
1	**Bikash Patra** National Institute of Science Education and Research, Bhubaneswar, India	Relevance of the Pauli kinetic energy density for semilocal functionals	Theory Development - Oral 1	OTD-1	Day 3 16th Dec. 2:30 pm IST (15 minutes)
2	**Dr. Igor Di Marco** Asia Pacific Center for Theoretical Physics, South Korea.	Determining the Intra-Atomic Exchange Energy in Rare-Earth Adatoms	Theory Development - Oral 2	OTD-2	Day 3 16th Dec. 2:45 pm (15 minutes)
3	**Aditi Mandal** Birla Institute of Technology and Science, Pilani, India	Brief description of Plasmon excitation within multiple scattering approach in Photoemission energy loss spectroscopy	Theory Development - Oral 3	OTD-3	Day 3 16th Dec. 3:00 pm IST (15 minutes)
4	**Dr. Subhayan Roychoudhury** Lawrence Berkeley National Laboratory, Berkley, USA	Neutral excitation density functional theory: a variational first-principles method for simulating excitations in molecules	Theory Development - Oral 4	OTD-4	Day 3 16th Dec. 3:15 pm IST (15 minutes)
5	**Santanu Pathak** Variable Energy Cyclotron Centre, Kolkata, India	Precision measurement and electronic structure calculations for understanding the microscopic and macroscopic properties of HfO_2	Theory Application -Oral 1	OTA-1	Day 3 16th Dec. 3:30 pm IST (15 minutes)
6	**Namrata Jaykhedkar** Faculty of Natural Sciences, Comenius University, Slovakia	Theoretical study of temperature dependent behaviour of crystal phases in $SrZrS_3$	Theory Application -Oral 2	OTA-2	Day 3 16th Dec. 3:45 pm IST (15 minutes)
7	**Shashi Bhusan Mishra** Indian Institute of Technology Madras, Chennai, India	Formation of a suspended magnetic layer between graphene layers through fluorine intercalation	Theory Application -Oral 3	OTA-3	Day 3 16th Dec. 4:00 pm IST (15 minutes)
8	**Dr. Tisita Das** Harish-Chandra Research Institute, Allahabad, India	Enhanced Hydrogen Evolution Activity at the Edges of $MPSe_3$ (M=Mn, Fe) Tri-chalcogenide Layers	Theory Application -Oral 4	OTA-4	Day 3 16th Dec. 4:15 pm IST (15 minutes)
9	**Abhishek Maiti** Indian Association for the cultivation of Science, Kolkata, India	Rashba Band Splitting in Methylammonium Lead Iodide: An Insight from Spin-Polarized Scanning Tunneling Spectroscopy	Experiment - Oral 1	OEX-1	Day 5 18th Dec. 4:50 pm IST (15 minutes)

10	**Sameer Kumar Mallik** Institute of Physics, Bhubaneswar, India	Hysteresis study in salt-assisted CVD grown monolayer MoS2 field-effect transistor by pulsed I~V technique	Experiment - Oral 2	OEX-2	Day 5 18th Dec. 5.05 pm IST (15 minutes)
11	**Dr. Rajib Batabyal** Center for Quantum Devices, Niels Bohr Institute, University of Copenhagen, Denmark	Topological Fermi-arcs and Weyl node connectivity in ferromagnetic Weyl semimetal $Co_3Sn_2S_2$	Experiment - Oral 3	OEX-3	Day 5 18th Dec. 5.20 pm IST (15 minutes)
12	**Dr. Sofi Suhail Majid** Institute of Physics, Academia Sincia, Taiwan	Unveiling the role of V-V dimerization on insulator-metal transition and optical transmittance of VO2 thin films	Experiment - Oral 4	OEX-4	Day 5 18th Dec. 5.35 pm IST (15 minutes)

EESTER 2020 – POSTER Presentations

SL. No	Name & Affiliation	Title	Category	Presentation Number	Schedule
1	**Sujoy Datta** Department of Physics, University of Calcutta, West Bengal, India	Semi-local DFT Advancement on Full Potential Localized Basis Scheme for Semiconductor Band-gap Prediction and Beyond	Theory Development - POSTER 1	PTD-1	Day 3 16th Dec. 4:50 pm IST (5 minutes)
2	**Dr. Nisha Singh**, Technical University Delft, Netherlands	Manipulation of magnon modes in alloys	Theory Development - POSTER 2	PTD-2	Day 3 16th Dec. 4:55 pm IST (5 minutes)
3	**Dr. Sri Kasi Matta**, RMIT University, Australia	Two-dimensional (2D) Transition metal chalcogenides (TcX_2, X=S, Se) for charge transport in Perovskite Solar Cells: A DFT study	Theory Application - POSTER 1	PTA-1	Day 1 14th Dec. 4:50 pm IST (5 minutes)
4	**Joydipto Bhattacharya**, Raja Ramanna Centre for Advanced Technology, Indore, India	Unusual magnetic and electronic properties of Al-substituted Ga_2MnNi: An ab initio study	Theory Application - POSTER 2	PTA-2	Day 1 14th Dec. 4:55 pm IST (5 minutes)
5	**Dr. Badiur Rahaman**, Aliah University, Department of Physics, IIA/27-Newtown, Kolkata, India	Electronic properties and microscopic modeling of Polymeric Fe(II) triazole	Theory Application - POSTER 3	PTA-3	Day 1 14th Dec. 5:00 pm IST (5 minutes)
6	**Saumen Chaudhuri**, IIT Kharagpur, West Bengal, India	Functionalization of monolayer MoS_2 by applying mechanical strain	Theory Application - POSTER 4	PTA-4	Day 1 14th Dec. 5:05 pm IST (5 minutes)
7	**Rajeev Dutt**, Raja Ramanna Centre of Advanced Technology, Indore, India	Probing the martenstie transition and thermoelectric properties of Co_xTaZ (Z=Si,Ge,Sn and x=1,2) : a study based on DFT	Theory Application - POSTER 5	PTA-5	Day 1 14th Dec. 7:10 pm IST (5 minutes)
8	**Aditya Shravan Shende**, Visvesvaraya National Institute of Technology (VNIT), S Ambazari Rd, Ambazari, Nagpur, Maharashtra, 440010, India	Exploration of Electronic and Topological Properties of Strain Induced Transition metal trichalcogenides Materials	Theory Application - POSTER 6	PTA-6	Day 1 14th Dec. 7:15 pm IST (5 minutes)
9	**Akshay Mahajan** Indian Institute of Technology Kanpur, Punjabi Mohalla Baharli Bundi, Bundi (Rajasthan) 323001, India	Strain-engineering-based study of 2D Multiferroic $VOCl_2$ Monolayer	Theory Application - POSTER 7	PTA-7	Day 1 14th Dec. 7:20 pm IST (5 minutes)

10	**Mandira Das**, Department of Physics, IIT Guwahati, Amingaon North Guwahati, Assam, India	Calculation of Quantum Capacitance and Pseudo-capacitance of Ti, Nb, Mo, V based Pristine and O-functionalized MXene using Density	Theory Application - POSTER 8	PTA-8	Day 1 14th Dec. 7:25 pm IST (5 minutes)
11	**Samarendra Roy**, Indian Institute of Technology, Kharagpur West Bengal 721302 Country: India	Effect of Mn on the precipitation kinetics of Al-Cu alloy	Theory Application - POSTER 9	PTA-9	Day 2 15th Dec. 4:50 pm IST (5 minutes)
12	**Mahendiran Durairaj**, CSIR-Central Electro Chemical Research Institute, Chennai, India	Understanding the Stability of Edge States in SiC Nanoribbons by First Principles Approach	Theory Application - POSTER 10	PTA-10	Day 2 15th Dec. 4:55 pm IST (5 minutes
13	**Halima Said**, Department of Physical and Theoretical Chemistry and Laboratory of Advanced Materials, Faculty of Natural Sciences, Comenius University, Ilkovicova 6, SK-84215 Bratislava, Slovakia	Ab-initio molecular dynamics study of cesiated molybdenum surfaces	Theory Application - POSTER 11	PTA-11	Day 2 15th Dec. 5:00 pm IST (5 minutes)
14	**Dr. Debolina Misra** Department of Metallurgical and Materials Engineering, IIT Madras, Chennai, India	Transition metal implanted oxide as support for noble metal single atoms	Theory Application - POSTER 12	PTA-12	Day 2 15th Dec. 5:05 pm IST (5 minutes)
15	**Rayan Chakraborty**, Indian Institute of Science Education and Research (IISER), Pune, India	Thermodynamics of Hydrogen Evolution from Surfaces of Earth-abundant Cu_2BaSnS_4	Theory Application - POSTER 13	PTA-13	Day 2 15th Dec. 7:30 pm IST (5 minutes)
16	**Marcelo Albuquerque**, Universidade Federal Fluminense (UFF), Brazil	XANES simulations in diamond-like two-dimensional material	Theory Application - POSTER 14	PTA-14	Day 2 15th Dec. 7:35 pm IST (5 minutes)
17	**Deepak S. Gaval**i, SRM University – AP, Andra Pradesh, India	Synergetic effect of localized and delocalized π electron on Li storage properties of Si/C heterostructures	Theory Application - POSTER 15	PTA-15	Day 2 15th Dec. 7:40 pm IST (5 minutes)
18	**Khorsed Alam** Harish-Chandra Research Institute. Chhatnag Road, Jhunsi, Prayagraj (Allahabad), Uttar Pradesh, India	DFT study into efficient bifunctional catalytic activity of cobalt dispersed N-doped graphitic nanospheres in Zn-air battery	Theory Application - POSTER 16	PTA-16	Day 2 15th Dec. 7:45 pm IST (5 minutes)

19	**Aswathi Mohan T** Institute of Science Education and Research (IISER), Pune, India	CO_2 capture, activation and dissociation on the Ti_2C surface and Ti_2C MXene: the role of surface structure	Theory Application - POSTER 17	PTA-17	Day 2 15th Dec. 7:50 pm IST (5 minutes)
20	**Aiswarya Samal** Indian Institute of Technology Bhubaneswar, Odisha, India	First principles study of strain effect on thermal and electrical transport of metal and graphene	Theory Application - POSTER 18	PTA-18	Day 2 15th Dec. 7:55 pm IST (5 minutes)
21	**Prince Gollapalli** Department of Metallurgical and Materials Engineering, Indian Institute of Technology, Madras, Chennai, India	On the Origin of Chemically Graded Metal/Ceramic Interface - A High Throughput DFT Study	Theory Application - POSTER 19	PTA-19	Day 3 16th Dec. 5:00 pm IST (5 minutes)
22	**V. Rajapandian** Department of Chemistry, Sri Ramakrishna Mission Vidyalaya College of Arts and Science, Coimbatore-641020, Tamil Nadu, India	Force Filed Parameters for Copper Proteins	Theory Application - POSTER 20	PTA-20	Day 3 16th Dec. 5:05 pm IST (5 minutes)
23	**Preeti Alhan** Department of Physics, Panjab University, Chandigarh, India	Electronic, half-metallic and magnetic properties of bulk Co_2TiGe Heusler alloy	Theory Application - POSTER 21	PTA-21	Day 3 16th Dec. 7:30 pm IST (5 minutes)
24	**Rohilla Dholpuria** Department of Physics, Panjab University, Chandigarh, India	Structural, Electronic and Elastic Properties of ScP at ambient pressure	Theory Application - POSTER 22	PTA-22	Day 3 16th Dec. 7:35 pm IST (5 minutes)
25	**Monirul Shaikh** Dept. of Physics and Nanotechnology, SRM Institute of Science and Technology, KTR, Tamil Nadu, India	Defect induced ferromagnetism in a two-dimensional metal–organic framework	Theory Application - POSTER 23	PTA-23	Day 3 16th Dec. 7:40 pm IST (5 minutes)
26	**Mukaddar Sk,** Dept. of Physics and Nanotechnology, SRM Institute of Science and Technology, KTR, Tamil Nadu, India	First-principles study on $Cs_2MM'Cl_6$ [M= Cu, Ag, Au; M'= Al, Ga, In, Tl] double perovskites halides for photovoltaic applications	Theory Application - POSTER 24	PTA-24	Day 3 16th Dec. 7:45 pm IST (5 minutes)

27	**M. J. Swamynadhan** Dept. of Physics and Nanotechnology, SRM Institute of Science and Technology, KTR, Tamil Nadu, India	Designing multifunctional two dimensional layered Van der Waals transition metal phosphorous chalcogenides	Theory Application - POSTER 25	PTA-25	Day 3 16th Dec. 7:50 pm IST (5 minutes)
28	**Goutam Paul**, School of Physical Sciences, Indian Association for the Cultivation of Science, Kolkata, India	Structure, Morphology, and Photovoltaic Implications of Halide Alloying in Lead-Free $Cs_3Sb_2Cl_xI_{9-x}$ 2D-layered Perovskites	Experiment -POSTER 1	PEX1	Day 5 18th Dec. 5:50 pm IST (5 minutes)
29	**Mrs. K. Safna**, Govt. polytechnic College, Chelakkara, Thrissur-680586, Kerala, India	Tailoring of optical band gap and microstructure profiling of vanadium based complex compound systems	Experiment -POSTER 2	PEX2	Day 5 18th Dec. 6:00 pm IST (5 minutes)
30	**Raja Chakraborty**, School of Physical Sciences, Indian Association for the Cultivation of Science, Jadavpur, Kolkata 700032, India	Dynamic Response of Alternating-Current-Driven Light-Emitting Diodes Based on Hybrid Halide Perovskites	Experiment -POSTER 3	PEX3	Day 5 18th Dec. 6:05pm IST (5 minutes)
31	**Pratap Pal**, Indian Institute of Technology Kharagpur, West Bengal-721302, India	Towards enhanced room-temperature photovoltaic effect in ferroelectric Bi and Fe codoped $BaTiO_3$	Experiment -POSTER 4	PEX4	Day 5 18th Dec. 6:10 pm IST (5 minutes)
32	**Priyaath Mal** Department of Pure and Applied Physics, Guru Ghasidas Vishwavidyalaya, Koni, Bilaspur-405009, India	Comparative Fermiology Study of $PbBi_2Te_4$ and $SnBi_2Te_4$ 3D Topological Insulators	Experiment -POSTER 5	PEX5	Day 5 18th Dec. 6:15pm IST (5 minutes)

Abstracts

Plenary Lectures

Theory of Electronic Structures from Experimental Results - The Anderson Way

G. Baskaran

IIT Madras, India, IMSc, Chennai, India & Perimeter Institute, Waterloo, Canada

P.W. Anderson (1923-2020) was a model builder par excellence in condensed matter physics. Body of experimental results and quantum chemistry helped him to write down non-trivial minimal models, to understand rich variety of properties of quantum matter. When faced with formidable challenges from his own models, he went back to nature, experimental results. It helped him to write down qualitatively correct mathematical solutions and offer new insights.

I will discuss Anderson's style of functioning and illustrate it with examples, some from my memorable journey with him into high T_c and other problems.

DFT and fundamentals of electronic structure calculations

Olle Eriksson

Department of Physics and Astronomy, Uppsala University, Uppsala, Sweden

In this talk the general ideas behind density functional theory will be given, and details will be given of how calculations of materials properties can be calculated from ab-initio theory. Recent directions in the use of density functional theory for finding new materials will also be discussed, and examples of predictions of new functional materials will be given. Finally, this talk will discuss briefly what material properties are most likely to be described well by this theory, and what properties are less reliably reproduced by theory, and why this is so.

Plenary Lecture 3

An introduction to photoelectron spectroscopy: How to estimate electronic parameter strengths from experiments

D. D. Sarma

Solid State and Structural Chemistry Unit, Indian Institute of Science, Bengaluru 560012, India

As the title suggests, I shall start with an elementary introduction to photoelectron spectroscopy, setting it in the larger context of various types of high-energy spectroscopies. Starting with what may be expected when applied to isolated atoms, I shall show how spectroscopic features reveal various electronic interaction strengths. Finally, I shall discuss the cases beyond atoms and introduce various approximations that may be employed to extract electronic parameter strengths relevant to describing the electronic structure of extended systems to the extent possible within the time limitations of this talk.

Adventures and discoveries in layered two-dimensional ferroelectrics

Sokrates T. Pantelides[1,2]
John Brehm[1], Lei Tao[1], Sabine M. Neumayer[3], Andrew Ohara[1], Petro Maksymovych[3], Nina Balke[3]

[1]Department of Physics and Astronomy, Vanderbilt University, Nashville, TN 37235 USA
[2]Department of Electrical Engineering and Computer Science, Vanderbilt University, Nashville, TN 37235 USA
[3]Center for Nanophase Materials Sciences, Oak Ridge National Laboratory, Oak Ridge, TN 37831 USA

Ferroelectricity, an analog of ferromagnetism entailing electrical instead of magnetic dipoles, has been investigated extensively since the 1980's for applications in memories, radiofrequency devices, low-power field-effect transistors, solar cells, and sensors/actuators. Transition-metal oxides have been the primary ferroelectric materials in thin-film form, but in the last few years, it has been recognized that layered ferroelectrics, bonded by weak van-der-Waals (vdW) interactions and thinned to nanoscale dimensions or even monolayer form offer significant advantages. This talk will start with an overview of standard ferroelectric behavior: spontaneous displacement of an ion sublattice in either of two equivalent directions results in an intrinsic polarization, which can be reversed (switched) by an external electric field. After a brief account of novel 2D ferroelectrics, the focus will be on the layered vdW ferroelectric $CuInP_2S_6$. This material has the unusual property of also being an ionic conductor, with the rare property that the same ions, in this case Cu ions, are responsible for both ferroelectric displacements and ionic conduction. The talk will describe a synergistic theory-experiment journey that led to a series of discoveries of extraordinary properties [1-3]: instead of the usual double-well potential for ferroelectric displacements, $CuInP_2S_6$ features a quadruple-well potential, corresponding to low- and high-polarization phases, with four polarization states; in addition to regular ferroelectric switching among these four states, an external electric field can also drive the Cu ions across the vdW gaps, signaling a polarization re-alignment *against* the applied electric field and unveiling a novel mechanism to realize negative capacitance; controlled electric-field pulses can trigger ionic currents through which one can exercise unique control of polarization switching. These unusual properties engender novel functionalities for diverse applications.

This work was supported by the U.S. Department of Energy, Office of Science, Basic Energy Sciences, Materials Science and Engineering grant DE-FG02-09ER46554 (theory at Vanderbilt University), through the Center for Nanophase Materials Science (experiments at Oak Ridge National Laboratory), and through the National Energy Research Scientific Computing Center (computations). All collaborators are identified and acknowledged in the author lists of the published papers [1-3].

1. J. A. Brehm et al. Nature Materials **19**, 43 (2020) .
2. S. M. Neumayer et al. Phys. Rev. Appl. **13**, 064063 (2020).
3. S. M. Neumayer et al. Adv, Energy Mater. **10**, 200172 (2020).

Plenary Lecture 5

Machine Learning Applied to Materials Science

Tamio Oguchi

ISIR-SANKEN, Osaka University, Japan

In recent years, the complexity and diversity of materials as the subject of research have increased not only from the demand for performance and cost, but also from that for the realization of a sustainable society related to environmental and energy issues. However, in many cases, it takes many years to put it into practical use as real materials or devices, and accelerating R&D has become an important issue. That's where data science came into being as the "fourth paradigm" following experimental, theoretical, and computational science. Data science is highly regarded as a method for accelerating R&D by constructing a mathematical model with predictability for a target problem based on a huge amount of accumulated information (big data). Machine learning is a typical method in data science, and model construction is realized by statistical procedures and evaluations. However, the current situation is that big data targeted by machine learning is rarely found in the field of materials science, and efforts to accumulate data utilizing first-principles calculations are being promoted in Europe and the United States. In this talk, I shall give an overview of these backgrounds and introduce our recent researches [1-4] by linking first-principles calculations and machine learning.

[1] T. Yamashita, N. Sato, H. Kino, T. Miyake, K. Tsuda, and T. Oguchi, "Crystal structure prediction accelerated by Bayesian optimization", Phys. Rev. Materials **2**, 013803 (2018).
[2] K. Terayama, T. Yamashita, T. Oguchi, and K. Tsuda, "Fine-grained optimization method for crystal structure prediction", npj Computational Materials **4**, 32 (2018).
[3] N. Sato, T. Yamashita, T. Oguchi, K. Hukushima, and T. Miyake, "Adjusting the descriptor for a crystal structure search using Bayesian optimization", Phys. Rev. Materials **4**, 033801 (2020).
[4] Y. Kanda, H. Fujii, and T. Oguchi, "Sparse modeling of chemical bonding in binary compounds", Sci. Tech. Adv. Mater. **20**, 1178 (2019).

Polymer Informatics: Current Status & Critical Next Steps

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The Materials Genome Initiative (MGI) has heralded a sea change in the philosophy of materials design. In an increasing number of applications, the successful deployment of novel materials has benefited from the use of computational, experimental and informatics methodologies. Here, we describe the role played by computational and experimental data generation and capture, polymer fingerprinting, machine-learning based property prediction models, and algorithms for designing polymers meeting target property requirements. These efforts have culminated in the creation of an online Polymer Informatics platform (https://www.polymergenome.org) to guide ongoing and future polymer discovery and design [1-3]. Challenges that remain will be examined, and systematic steps that may be taken to extend the applicability of such informatics efforts to a wide range of technological domains will be discussed. These include strategies to deal with the data bottleneck, new methods to represent polymer morphology and processing conditions, and the applicability of emerging AI algorithms for materials design.

[1] Rohit Batra, Le Song and Rampi Ramprasad, “Emerging materials intelligence ecosystems propelled by machine learning”, *Nature Reviews Materials* (2020)

[2] Huan Doan Tran, Chiho Kim, Lihua Chen, Anand Chandrasekaran, Rohit Batra, Shruti Venkatram, Deepak Kamal, Jordan P. Lightstone, Rishi Gurnani, Pranav Shetty, Manav Ramprasad, Julia Laws, Madeline Shelton, and Rampi Ramprasad, “Machine-learning predictions of polymer properties with Polymer Genome”, *Journal of Applied Physics* (2020).

[3] A. Mannodi-Kanakkithodi, A. Chandrasekaran, C. Kim, T. D. Huan, G. Pilania, V. Botu, R. Ramprasad, “Scoping the Polymer Genome: A Roadmap for Rational Polymer Dielectrics Design and Beyond”, Materials Today, 21, 785 (2018).

Prof. Ramprasad is presently the Michael E. Tennenbaum Family Chair and Georgia Research Alliance Eminent Scholar in the School of Materials Science & Engineering at the Georgia Institute of Technology. His area of expertise is the development and application of computational and machine learning tools to accelerate materials discovery, as applicable to energy production, storage and utilization. Prof. Ramprasad received his B. Tech. in Metallurgical Engineering at the Indian Institute of Technology, Madras, India, an M.S. degree in Materials Science & Engineering at the Washington State University, and a Ph.D. degree also in Materials Science & Engineering at the University of Illinois, Urbana-Champaign.

Prof. Ramprasad is a Fellow of the Materials Research Society, a Fellow of the American Physical Society, an elected member of the Connecticut Academy of Science and Engineering, and the recipient of the Alexander von Humboldt Fellowship and the Max Planck Society Fellowship for Distinguished Scientists. He has authored or co-authored over 225 peer-reviewed journal articles, 8 book chapters and 8 patents, and has delivered over 300 invited talks at Universities and Conferences worldwide. He is a member of the Editorial Advisory Boards of ACS Materials Letters and Journal of Physical Chemistry A/B/C, and is the Chair of the inaugural 2022 Gordon Research Conference on Computational Materials Science and Engineering.

Atomic Scale Imaging and Spectroscopy with Aberration Corrected Transmission Electron Microscopy

Joachim Mayer

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and
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The invention of aberration correctors has revolutionized the development of TEM and STEM instrumentation. Only shortly after the development and installation of the first TEM with a corrector for the spherical aberration, commercial instruments with aberration correctors have been introduced by all major manufacturers. In order to provide a platform for these novel developments and based on the experience with the first aberration corrected TEM, Research Centre Juelich and RWTH Aachen University have jointly founded the Ernst Ruska-Centre for Microscopy and Spectroscopy with Electrons (ER-C). At the Ernst Ruska-Centre we have recently installed the FEI Titan 60-300 PICO. PICO is a fourth-generation transmission electron microscope capable of obtaining high-resolution transmission electron microscopy images approaching 50 pm resolution in the C_C- and C_S-corrected mode at 300 keV. It is currently one of only three microscopes in the world capable of chromatic aberration correction. In my lecture, I will explain the basics of aberration corrected TEM and will then outline how it has improved the possibilities and accuracies of measurements on the atomic scale. Based on electron energy loss spectroscopy (EELS) and energy filtering TEM (EFTEM), spectroscopic experiments can give quantitative insight in further materials properties. Analysing the energy loss near edge fine structure (ELNES), the electronic band structure can be analysed with near atomic resolution. In this way, valency states and bonding can be analysed at defects an interfaces and the results can be correlated with the functional properties.

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Joachim Mayer received his Ph. D. in Physics at the Max-Planck-Institut für Metallforschung, Stuttgart, Germany. In 1988 he joined the Materials Department at the University of California, Santa Barbara, as a postdoctoral research associate. In 1990 he moved back to the Max-Planck-Institut für Metallforschung, Stuttgart, where he worked as a research scientist and Group Leader 'Analytical Electron Microscopy'. In 1999 he joined RWTH Aachen University to become Professor and Head of the Central Facility for Electron Microscopy of RWTH Aachen. In 2004, he received a co-appointment as one of the two directors of the newly founded Ernst Ruska-Centre at Research Centre Juelich.

Complex magnetic order and their spontaneous spin and charge currents

Lars Nordström

Department of Physics and Astronomy, Uppsala University, Uppsala, Sweden

We will discuss the origin and nature of complex magnetically ordered states, among which we will focus on non-collinear order in bulk materials often in the presence of non-negligible spin-orbit coupling, with examples of materials such as Sr_2IrO_4 and Mn_3Sn but also fcc Fe. They will be discussed based on their symmetries and their realistically calculated electronic structure. For instance, some focus will be put on the spin and charge currents that occur spontaneously in these systems, both due to the non-collinear order and the spin orbit coupling. As ordinary density functional theory often has short-comings to properly describe these effects we will outline a DFT+U formalism that bring tools to better understand them. In order to understand the origin of these orderings we will also outline a way to map the properties of these materials onto spin models that take proper account of the spontaneous currents, which play an important role.

Topological superconductivity and Majorana fermions

Annica Black-Schaffer

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Topological superconductors with Majorana fermion quasiparticles form a newly discovered class of matter. The Majorana fermion can be seen as half an electron, or more accurately, the electron wave function has split up into two completely separate parts. I will explain the basic physics behind topological superconductors, and how they are connected to topological insulators, as well as why Majorana fermions appear, before briefly reviewing the current experimental status and reporting a few of our recent findings.

Abstracts

Workshop Lectures

DFT in condensed systems : some practical guidelines

G.P. Das
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DFT has proved itself to be extremely handy tool in understanding the physical and chemical properties of materials from bulk to nano, and also in designing novel materials with desired combination of properties. This talk is aimed at providing an overview of the techniques being used to solve the Kohn-Sham (KS) equation with suitable exchange-correlation potentials to explore various kinds of materials and their properties. The two broad categories of KS-DFT implementations viz. pseudo-potential methods based on plane waves and all-electron methods based on localized augmented basis functions, have their respective strengths and weaknesses. The precision with which one can estimate various properties from these codes, as well as their accuracy to validate with the corresponding experimental results, have been studied extensively. While plane-wave based methods are being widely used for tackling a large variety of problems, atom-centered (spatially localized) energy dependent basis functions combine efficiency with accuracy, and also helps extracting the chemical information of a condensed system in a transparent way. I shall try to give a 'guided tour' of these practical aspects of DFT calculations for real materials. Finally, the target audience for this talk will be Masters / PhD students, young researchers (including experimentalists who are desirous of using DFT codes) who want to have a working knowledge for using DFT based electronic structure methods, and also want to understand their capabilities and limitations.

Brief Bio-sketch:

Prof. G.P. Das is a condensed matter physicist and a materials scientist working as Visiting Professor in IIT Kharagpur. He specializes in first-principles simulation and design of materials from bulk to nano, with specific applications in materials science and nano-devices. He has used density functional based approach to calculate the electronic, magnetic, and thermodynamic properties of intermetallic alloys, epitaxial interfaces, multilayers, clusters, and low dimensional quantum structures. Prof. Das served as visiting scientist/faculty in a number of institutes viz. MPI Stuttgart, VCU Richmond, IMR Sendai, UNSW Sydney. He has also spearheaded several research programmes nationally and internationally.

Broken symmetry driven topological semi-metal to gaped phase transition in SrAgAs

Aftab Alam[1], C Mondal[2], C K Barman[1] and B Pathak[2]

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Abstract

We show the occurrence of Dirac, Triple point, Weyl semimetal and topological insulating phase in a single ternary compound using specific symmetry preserving perturbations. Based on first principle calculations, symmetry analysis and *k.p* model, we show that alloy-induced symmetry breaking in SrAgAs (space group $P6_3mc$) helps to tune various low energy excitonic phases transforming it from Dirac to topological insulating state via intermediate triple point phase. We also consider the effect of external magnetic field, causing time reversal symmetry (TRS) breaking, and analyze the effect of TRS towards the realization of Weyl state. Topological insulating nature is further confirmed by calculating Z_2 index. Topologically protected surface states and Fermi arcs are also investigated in some detail. Most importantly, in this material, the Fermi level lies close to the nodal point with no extra Fermi pockets. This, in turn, makes these compounds an ideal platform to pave a path for experimentalists and verify the theoretical findings with appropriate probe. Such discovery of new candidate materials using alloy engineering is extremely useful to guide further design of topological quantum materials.

References:

[1] C Mondal, C K Barman, Alam et al., Phys. Rev. B 99, 205112 (2019)
[2] QuanSheng Wu et al., Phys. Rev. B 98, 081115(R) (2018).

Modeling Strongly Correlated Systems

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In this talk, we shall describe in details the key ingrediants that are necessary to model strongly correlated systems. In particular, we shall illustrate the derivation of low energy tight-binding model Hamiltonian using the downfolding method that serve as the single electron part of the Hubbard and Kanamori Hamiltonians. We shall show in the strong coupling limit, we can derive spin models, eg. Heisenberg model and in the presence of strong spin-orbit coupling the Kitaev model. Finally we shall illustrate such models with built in chemical realism help us to understand a large class of quantum materials.

Spectroscopy for electronic structure analysis

Kalobaran Maiti
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Electron spectroscopy, a technique based on photoelectric effect, directly probes the electronic structure of a material that derives the material properties. This is an ideal technique to reveal underlying physics of material properties such as superconductivity, magnetism, topological phases of matter etc. Employing high resolution photoemission spectroscopy, we have found some interesting scenario in various novel materials. Normally, density wave states (CDW/SDW) is found in a metal having finite number of electrons at the Fermi level. However, experiment shows such states even in insulators. We discovered that such unusual charge density wave states/giant anomalous transport can also happen due to localized electrons at the Fermi level. Impurities and/or vacancies in a material can lead to ferromagnetism with high transition temperature even in a non-magnetic material. Surface states of a topological insulator can be influenced by the adsorbed surface impurities. We exploited the polarization of the pump pulse in a time-resolved measurement to selectively excite electrons of different orbital character in Fe-based systems and discover that one can selectively heat electrons of a particular character without affecting other electrons. This method provides a way to disentangle parameters responsible for exoticity in a material.

Proximity-Induced Superconductivity in Epitaxial Quantum Spin Hall Heterostructures

Bent Weber

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The interplay of topology and superconductivity in condensed matter has become a subject of intense research for its importance in realising and advancing Majorana based topological quantum computing. Atomically thin (2D) topological materials – such as the quantum spin Hall (QSH) insulator – are emerging as promising candidate materials due to the possibility to combine them in high-quality epitaxial van-der-Waals heterostructures. We show that both can be achieved in van-der-Waals heterostructures of the QSH insulator 1T'-WTe_2 and the layered type-II superconductor 2H-$NbSe_2$, synthesized in low-temperature van-der-Waals molecular beam epitaxy (MBE). Using scanning probe spectroscopy (STS) down to 500mK, we confirm a QSH normal state in the topological heterostructure, with a bulk gap ~70meV at the Fermi level and metallic edges that show signatures of a highly-correlated 1D electron liquid in the normal state. Describing the functional form of the induced superconducting energy gap in a multi-band framework, we take the particularities of the $NbSe_2$ substrate explicitly into account and extract a pairing amplitude as large as 0.6 meV induced in WTe_2.

Novel states in magnetism: low-dimensional systems and spin liquids

Avinash V. Mahajan

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In systems with low magnetic dimensionality and low spin, quantum fluctuations play a dominant role and prevent long-range order, especially in one dimension. Their ground states are novel as are the excitations. I will review the experimental manifestations of such novel properties and contrast them with what is seen in conventional ferromagnets/antiferromagnets. Even in higher dimensions, one can evade long-range order by having conflicting magnetic interactions. Systems which do not order even at T = 0, in spite of strong magnetic interactions, have been called Quantum Spin Liquids (QSL). QSL possess various kinds of long-range entangled ground states which are said to have topological order. Such states also have emergent quasiparticles which exhibit exotic properties. One route to realize QSL is through geometric frustration (as suggested first by P.W. Anderson for triangular geometries). Several frustrated lattices such as Kagome (corner-shared triangles), hyperkagome, pyrochlore, etc. have been investigated and clear indications of QSL have been seen. Emergent excitations which follow fractional statistics have been proposed leading to some predictions about behavior of physical quantities which can be observed in experiments. A recent development in QSL is the prediction of QSL in the Kitaev model (KSL). I will review the progress in the experimental realisation of QSL/KSL.

Abstracts

Seminar Lectures

Seminar Lecture 1

Microscopic origin of near room-temperature multiferroic phenomena in $(LuFeO_3)_m/(LuFe_2O_4)_1$ superlattices

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Research in the field of multiferroics was initially stimulated by a quest for mechanisms of accommodating multiple ferroic properties in a single material. In recent years, the focus of research in this direction has turned towards discovering suitable materials that exhibit multiferroic properties and strong cross coupling among various ferroic phenomena at room temperature. Recently, the superlattices $(LuFeO_3)_m/(LuFe_2O_4)_1$, consisting of strong geometric ferroelectric $LuFeO_3$ layers and charge ordered ferrimagnetic $LuFe_2O_4$ layers, were found to exhibit multiferroic and magnetoelectric phenomena near room temperature. We shall discuss the microscopic origin of these phenomena in these superlattices on the basis of our research premised on the first-principles electronic structure calculations, materials specific spin Hamiltonian and finite temperature simulations [1,2].

[1] Julia A. Mundy,……,**Hena Das** *et.al.* Nature **537**, 523-527 (2016).
[2] Shiyu Fan, **Hena Das** *et. al.* Nature Communications **11**, 5582 (2020).

Seminar Lecture 2

Multiferroic Properties and Unconventional Spin Density Wave in Doubly Ordered Perovskite Na*Ln*NiWO$_6$ (*Ln*=Y, Dy, Ho, and Yb)

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Type-I multiferroics are polar magnetic insulators where the electric polarization comes from the displacement of ions due to chemical bonding or polyhedral distortion, and the magnetism is associated with the partially filled transition metal ions. Here, we present multiferroicity in Na*Ln*NiWO$_6$ (*Ln*=Y, Dy, Ho, and Yb), where the ferroelectricity results from a combined effect of chemical ordering octahedral distortion and the low-temperature magnetic order of Ni^{2+} ions. We also report an unconventional spin density wave occurring just below.

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NANO-ELECTRODES FOR ULTRAFAST DNA SEQUENCING

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The prospect of finding an improved method for rapid genome sequencing might offer a completely new way of preventive health care. Recently solid-state nanopores have generated lot of interest for ultrfast DNA sequencing. However, there are challenges to slow down the DNA translocation process to achieve a single-nucleobase resolution. We have used a range of computational tools in an attempt to study the DNA translocations in several model systems. Functionalizations [1-2] of electrodes are done to achieve a single-nucleobase resolution.

Here we will present a critical overview of some of the benefits that the covalent attachment of various probe molecules might offer in the context of DNA sequencing with nanopore-embedded electrodes.

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Hybrid organic-inorganic perovskites (HOIPs) are introducing new directions in the photovoltaic materials landscape

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The coexistence of inversion symmetry breaking and spin-orbit interactions play a key role in their optoelectronic properties. In this talk, we will discuss the interplay of electrical ordering and spin-related coupled properties starting from simple perovskite halides to a complex and recently synthesized ferroelectric layered HOIP, (AMP)PbI_4 (AMP = 4-aminomethyl-piperidinium). In the last case, we report a striking new effect, i.e., an extraordinarily large Rashba anisotropy that is tuneable by ferroelectric polarization: as polarization is reversed, not only the spin texture chirality is inverted, but also the major and minor axes of the Rashba anisotropy ellipse in k-space are interchanged, i.e. a pseudo rotation. A kp model Hamiltonian and symmetry-mode analysis reveal a quadrilinear coupling between the cation-rotation modes responsible for the Rashba ellipse pseudo-rotation, the framework rotation, and the polarization.

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Topological phases of matter

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Topological phases are defined by mapping the wavefunctions or fields from the position space to the topological spaces. Despite their material realizations, their material flexibility for applications has remained a grant challenge. In this talk, I will start with the introduction to the topological band theory. Then, I will discuss how to computationally engineer various topological phases by stacking different layered materials with opposite spin-orbit coupling, or via twisting bilayers.

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Descriptor to define the activity of carbon catalyst for OER: Quantum Mechanics and Machine Learning Approach

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Oxygen evolution reaction (OER) is a key aspect of energy conversion and storage technologies. The optimal electrocatalyst can speed up the sluggish kinetics of OER. **It is important to understand the energy parameter 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, high surface area, low cost, abundant etc. **The task is mammoth to find the best carbon catalyst in large material space but can be done through identification of correct features and subsequently using of machine learning tools**.

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. Machine learning algorithms like Multiple Linear Regression, Random Forest Regression and Support Vector Regression (SVR) are trained on the data generated by density functional theory to predict the overpotential. An optimal active site for OER using proposed SVR model is identified with overpotential (0.29V) and then validate through DFT calculations. To generalize the study, we used SVR model on N doped GNR to predict the site-specific activity towards OER.

The work is done with
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Deep Learning and Active Learning of Interatomic Force Fields

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Molecular dynamics simulation with predefined functional forms is a popular technique for understanding dynamical evolution of systems. These predefined functional forms of interatomic force fields impose limits on the physics that can be captured. In this direction, deep learning models such as a Deep Neural Network (DNN) has emerged as an attractive flexible alternative in the area of molecular force-fields. The DNN models are trained against DFT (density functional theory) data, and, ideally, if one is able to train a DNN to accurately predict the correct DFT energy and forces for any given structure, they gain the ability to perform molecular dynamics with high accuracy while simultaneously reducing the computation cost in a dramatic fashion. While this goal is very lucrative, neural networks are interpolative and therefore, it is not always clear how one should go about training a neural network to exhaustively fit the entire phase space of a given system. Currently, DNNs are trained by generating large quantities (on the order of 10^4 or greater) of training data in hopes that the DNN has adequately sampled the energy landscape both near and far-from-equilibrium. This can, however, be a bit prohibitive when it comes to more accurate levels of quantum theory. As such, it is desirable to train a model using the absolute minimal data set possible, especially when costs of high-fidelity calculations such as CCSD and QMC are high. Here, we present an active learning approach that iteratively trains an ANN model to faithfully replicate the energy surface of water and gold using minimal number of total structures (~500) in its training data. We also demonstrate that molecular dynamics simulations based on such actively learned DNN models are able to capture thermophysical properties very accurately.

Defect induced emergent phenomena at the surface and interface of band insulators

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Predictive control over defect minimization is the most important aspect during growth of any material. While it is undesirable to have defects in the system, it very often leads to unexpected modulation of physical properties which could have marked technological applications. Such is the case with complex oxides where oxygen vacancies (OVs) are the most common point defects. In the first part of the talk, OV induced emergent phenomena in a non-magnetic band insulator $KTaO_3$ (KTO) will be discussed. Creation of OV in (001) oriented single crystals of KTO makes it a metal. Unexpectedly, oxygen deficient KTO shows signature of topological Hall effect (THE). Ab initio calculations reveal simultaneous formation of the magnetic moment on Ta atoms around an isolated OV and Rashba-type spin texturing of conduction electrons. In the presence of Rashba SOC, the local moments around vacancy can form bound magnetic polarons with noncollinear spin texture, resulting in THE.

In the second part of the talk, the effect of electrostatic gating on transport properties of the conducting interface between two band insulators γ-Al_2O_3 and $SrTiO_3$ (STO) will be presented. The conductivity in this heterostructure primarily originates from the presence of excess OVs. Our transport measurements reveal enhancement in clustering of OVs in presence of electric field. This leads to time dependent charge trapping phenomena which can continue for several hours. Most importantly, we detect an additional source of charge trapping (detrapping) at (from) ferroelastic twin walls of STO. The amount of trapped/detrapped charges at the twin wall is electric field tunable and is controlled by the net polarity of the wall. These trapped charges at the twin walls would act as localized magnetic moments and can result in electric field tunable unconventional magnetic phases in STO based heterostructures.

Role of Disorder, Spin Orbit Coupling and Magnetism in the Electronic Structure of Ir Based Double Perovskite

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Transition metal oxide based double perovskites are a playground for understanding the role of disorder on the physical properties. In this talk, I will present the electronic structure of Iridium based disordered double perovskite Sr_2TiIrO_6 studied using photoemission spectroscopy. Transport and magnetic properties will be discussed. Ab-initio band structure calculations will be presented to understand the role of electron correlation and the spin orbit coupling in the electronic structure. High resolution valence band photoemission across the magnetic transition will also be presented to unravel the role of magnetism and disorder in the electronic structure of correlated disordered system.

Atomic scale experimental characterization complimented by atomic scale simulations for component scale materials designing

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The presentation will deal with examples of materials design where atomic scale simulations were utilised to an extent unprecedent in the many sense. The first example concerns with development of high temperature age hardenable cast Aluminum alloys which should bear adequate strength at operating temperatures ≥300°C, yet should limit the cost within the range of present stakeholders. The main obstacle was the rapid coarsening of nano-scale strengthening θ'precipitates which results in rapid degradation in load bearing capacity at such high temperatures. The coarsening was related to the semi-coherent and thereby mobile matrix-precipitate interface. The solution to rapid coarsening was therefore to design the interface chemistry such that the coherency strain diminishes. This was carried out by a unique combination of experimental (atomic level elemental characterization using atom probe tomography, APT) and simulation (atomic scale density functional theory, DFT) tools. The results indicated the role of several elements like Mn and Zr to stabilize the semi- coherent interface by preferential segregation. This information was then used to develop the target alloy composition to make actual automobile parts (cylinder heads).

The second example addresses the issue of atomic scale spatial distribution of substitutional alloying elements (Al and V) and interstitial impurities (O, N and C) in Ti-6Al-4V alloy. Here also, elemental characterization by APT were substantialised by DFT simulations which indicates preferential segregation of interstitial impurities (like O, C and N) along microstructural regions within the α-phase. Amongst the substitutional alloying elements, Al shares inverse interrelation with Oxygen while V-atoms reside besides impurity-rich regions.
The specific importance of these findings is that enrichment of interstitial impurities within the α-phase has shown to change the fracture mode from ductile to cleavage-in Ti-6Al-4V alloy. The study explains as to why such segregation would occur in the first place. It also helps to design alloy compositions with balanced interstitial and substitutional elemental concentrations such that the components have superior mechanical properties like higher ductility and longer fatigue life.

At the end, a similar design concept, yet to be applied though, will be discussed for a mica-based machinable glass-ceramics system. Machinability here stems from two sources, (a) the weak mica crystal/residual base glass interfaces and (b) preferential cleavage fracture of mica crystals along the (001) basal planes. Understanding the crystal-glass interface is therefore the key to understand the root of crack deflection, fracture resistance and related machinability in these glass-ceramics. For this end, elemental characterization by APT complimented by DFT simulations will be utilized to understand the composition of the interfaces which should help to engineer them and push the limit further by designing newer glass-ceramics compositions. This should also lead to the generalization of machinability by developing several such machinable glass ceramics or for the matter, making any glass ceramics machinable through interfacial engineering.

Abstracts

ORAL Presentations
Theory Development (OTD)
Theory Application (OTA)
Experiment (OEX)

Relevance of the Pauli kinetic energy density for semilocal functionals

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A meta-generalized gradient approximation (meta-GGA) exchange functional, based only on the Pauli kinetic enhancement factor, is constructed for quantum chemistry and solid- state physics. The underlining construction of this exchange energy functional is based on a nonlinear equation found from a generalization of the Becke-Roussel approach, where we use the cuspless hydrogen exchange hole density model. We combine the meta-GGA exchange with a simple GGA correlation. The resulting exchange-correlation semilocal functional is remarkably accurate for several thermochemical test cases and quite efficient for the structural and energetic properties of bulk solids. It also provides, in the generalized Kohn-Sham scheme, better orbital energies of atoms and band gaps of semiconductors than other popular semilocal functionals. Recently, it is shown the proposed meta-GGA functional is very promising for band gaps of doped graphene, graphane, and halogenated graphene having insulating gaps. Also, our recent calculation shows that this functional gives better structural stability of challenging solid-state systems including FeS2, TiO2 and MnO2. The present construction is showing the high relevance of the Pauli kinetic energy density for the functional development.

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Determining the Intra-Atomic Exchange Energy in Rare-Earth Adatoms

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Abstract

In this presentation, I will report on our joint theoretical and experimental study of the intra-atomic exchange energy between the inner *4f* and the outer *6s5d* shells in rare-earth elements [1]. Inelastic electron tunneling spectroscopy on individual rare-earth atoms adsorbed on metal-supported graphene reveals an element-dependent excitation, with energy between 30 and 170 meV, linearly increasing with the spin angular momentum of the *4f* shell. This observation is possible owing to the strong spin polarization of the outer shells, characteristic of rare-earth adatoms on graphene. This polarization gives rise to a giant magnetoresistance of up to 75% observed for Dy on graphene/Ir(111) single-atom magnets. Density functional theory calculations of the *6s5d* shell spin polarizations and of their intra-atomic exchange constants with the *4f* shell yield exchange energies in agreement with the experimental values. These results prove that the description of the spin dynamics in RE considering only the *4f*−*5d* interaction is oversimplified. A more realistic treatment requires us to consider a multishell intra-atomic exchange in which both *6s* and *5d* shells are taken into account, with the *4f*−*6s* contribution possibly prevailing over the *4f*−*5d* one. Our findings not only represent the first direct determination of intra-atomic exchange energy, but are also important for the general understanding of magnetism in rare earths, whether they are in bulk compounds or as surface adsorbed atoms and clusters.

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OTD3

Brief description of Plasmon excitation within multiple scattering approach in Photoemission energy loss spectroscopy

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Photoemission energy loss spectroscopy (PEELS) aims at providing information on the dielectric function near the surface. Basically, it consists in the monitoring of a plasmon satellite in a photoemission spectrum as a function of the direction of the outgoing electron that has suffered a plasmon loss. In order to be able to derive quantitative information on the (surface) dielectric function, a comparison with suitable theoretical model is necessary upon which we are working presently. Our aim is to develop such theoretical model for 3D as well as 2D materials and incorporate it into a computer code MsSpec[1].

The plasmon loss will be described within the so-called quasi-boson approximation, originally proposed by Hedin [2] and further extended by Fujikawa [3]. We use this electron-boson Hamiltonian (Eq.1), where both the photoelectron and the core electron are coupled to bosonic-type excitations in the solid:

$$H = \sum_{q} \omega_q a_q^\dagger a_q + \sum_{k} \varepsilon_k c_k^\dagger c_k + \sum_{qkk'} V_{kk'} (a_q + a_q^\dagger) c_k^\dagger c_{k'} \tag{1}$$

Both Hedin and Fujikawa approaches rely on a specific fluctuation potential (the potential which describes the excitation of a plasmon), approximating the core state wavefunction by a delta function without considering multiple scattering of the outgoing electron after the excitation of the plasmon, which is important for interpretation of data for various spectroscopies[4]. We compared the different fluctuation potentials i.e. Plasmon-pole, Bechstedt and other available potentials and will use either the exact core state wave function or a model, more accurate than a simple delta function[5]. Further a fully quantum description of plasmons involves an accurate calculation of the dielectric function which contains the many-body response of the system, including plasmons and their interactions with other (quasi-)particles, which control their lifetime and their decay channels. So, we use the quantum many-body method of Fermi liquids to model the dielectric function and its behaviour under external fields. Thus further, to calculate the dielectric function accurately, we approximate the exact fluctuation potentials by model numerical fluctuation potentials. We will present our results with different such model fluctuation potentials that have been proposed in the literature alongwith the calculated ones from the dielectric function which incorporates plasmon dispersion from hydrodynamic to random phase approximation (RPA) and beyond improving with static and dynamical local field corrections. Presently the model is for one plasmon and we will extend it to two, three plasmons. The model calculations are being tested for Aluminium target.

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OTD4

Neutral excitation density functional theory: an efficient andvariational first-principles method for simulating neutral excitations in molecules

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We introduce neutral eXcitation Density Functional Theory (XDFT), a computationally light, generally applicable, first-principles technique for calculating neutral electronic excitations in finite systems. The concept is to generalise constrained density functional theory (cDFT) to free it from any assumptions about the spatial confinement of electrons and holes, but to maintain all the advantages of a variational method. Within the Kohn-Sham framework, XDFT simulates the lowest excitation of an electron of spin σ by performing variational energy minimization in conjunction with a constraint-condition Tr[$\hat{\rho}^{\sigma}\hat{\mathrm{P}}$] = $N^{\sigma} - 1$, where $\hat{\rho}^{\sigma}$ is a spin-dependent density operator, N^{σ} is the number of σ-spin electrons in ground state and $\hat{\mathrm{P}}$ is the projection operator on the ground state occupied subspace of spin σ. This ensures that in the neutral excited state, a single σ-spin electron is confined outside the subspace given by $\hat{\mathrm{P}}$. The task of calculating the lowest excited state of a given symmetry is thereby simplified to one of performing an inexpensive sequence of coupled DFT calculations. We demonstrate the efficacy of the method by calculating the lowest single-particle singlet and triplet excitation energies in the well-known Thiel molecular test set, with results which are in good agreement with linear-response time-dependent density functional theory (LR-TDDFT). Furthermore, we show that XDFT can successfully capture two-electron excitations, in principle, offering a flexible approach to target spe- cific effects beyond state-of-the-art adiabatic-kernel LR-TDDFT. We also establish the connections between XDFT and the exact theorems for excited state DFT. Overall the method makes optical gaps and electron-hole binding energies readily accessible at a computational cost and scaling comparable to that of standard density functional theory. Owing to its multiple qualities beneficial to high-throughput studies where the optical gap is of particular interest; namely broad applicability, low computational demand, and ease of implementation and automation, XDFT presents as a viable candidate for research within materials discovery and informatics frameworks.

Further details : Roychoudhury, S.; Sanvito, S.; O'Regan, D. D., Sci. Rep. 2020, 10, 8947

Abstract for EESTER 2020

Precision measurement and electronic structure calculations for understanding the microscopic and macroscopic properties of HfO_2

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Studies on electronic and structural properties of Hafnia (HfO_2) has remained as a topic of interest as this material exhibits exotic properties and thus having immense application potential [1]. So, experimental studies continued and electronic structure calculations were performed simultaneously for understanding these properties. It was known that HfO_2 shows polymorphism, but the experimental reports showed a large variation in the pressure value for the transformation from ambient monoclinic ($P2_1/c$) to orthorhombic-I phase to occur. A recent study on pressure-induced structural change using synchrotron X-ray diffraction technique along with Density functional calculations revealed that the orthorhombic-I phase transformation is observable at ~3.7 GPa and the transition is adiabatic in nature [2].

Recently, HfO_2 has attracted special attention after ferroelectric property was observed [3]. As first principle calculations indicated two orthorhombic polar phases (space groups $Pca2_1$ and $Pmn2_1$) most viable ferroelectric phases of Hafnia [4], extensive studies were performed with different dopants in search for ferroelectric property in HfO_2. Interestingly, it is observed that a minimal doping of 1% Ta in HfO_2 initiates phase transformation from monoclinic ($P2_1/c$) to orthorhombic phase under ambient conditions [5]. Surprisingly, the percentage of phase transformation increases with increasing the dopant concentration upto 10%. Further increase in the dopant concentration reduces the proportion of phase transformation in HfO_2 compared to the monoclinic phase which continues to exist. The Ta-doped samples studied at high pressure conditions using synchrotron beam revealed a saturation effect in the percentage of phase transformation.

A precision study on crystal structure of HfO_2 was performed using synchrotron and neutron diffraction techniques [6]. The position of the constituent oxygen (O) atoms could be measured with a higher precision using neutron diffraction technique and electronic structure calculations were performed using them as inputs. It is observed that the hybrid functionals, viz. B3LYP, HSE06 or hybrid functional based TB-mBJ approach do not take care of the precise information regarding structural parameters in terms of electronic band gap. Rather, the work supports the observation that semi-local functional better describe the oxides.

In this study, first-principles calculations have been performed within density functional theory (DFT) framework to calculate the electric field gradient (EFG) using the precision structural parameters of HfO_2 obtained experimentally. Electric Field Gradient (EFG) is a microscopic parameter which describes the asphericity in the electron density in the vicinity of nucleus [7]. This microscopic parameter is obtained from hyperfine interaction studies where quadrupole moment (Q) of the nucleus interacts with the EFG. Quarupole frequency (ω_Q) is measured using techniques like, TDPAC, Mössbauer spectroscopy etc. and EFG is evaluated from that measured quantity with a known value of Q. The EFG parameter is very sensitive to local structural changes as it varies with the distance of the charge density from the probe nucleus (r) as $1/r^3$. So, precise structural parameters play the key role in the evaluation of EFG which provides information about the electronic structure around the probe nuclei.

We performed calculation with the PBE-GGA exchange correlation functional after one out of 4 Hf-atoms in an HfO_2 unit-cell replaced with a Ta-atom as shown in Fig 1. This introduction of Ta makes the cell charged (q=+1). From the calculation using the precise structure, we obtain EFG (V_{ZZ}) = 12.95×10^{21} V/m^2, where V_{ZZ} is the major component of the EFG tensor. This value is in agreement with the experimental value that ranges from 12.8 to 13.2 $\times 10^{21}$ V/m^2[8-10]. It was observed that relaxation of the atoms changes the Ta-O distance negligibly. Alonso *et al.* calculated value of EFG at the Ta-site reported using the experimental values and after taking a relaxed structure of HfO_2 in a 96-atom cell and obtained 13.7 $\times 10^{21}$ V/m^2 [11]. As Alonso *et al.*'s work was based on structure of HfO_2 derived from X-ray diffraction technique only, precise oxygen position was not available. The change in the electronic environment and thus the contribution of p-electrons obtained after considering precise position of the constituent O-atom will be discussed.

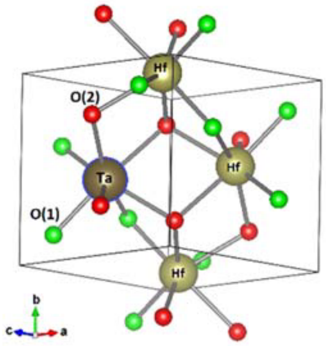

Figure 1: Unit-cell of HfO_2 with one Hf-atom replaced with Ta-atom. The crystal consists of Hf and 2 non-equivalent O-atoms; O(1) is marked with green and O(2) with red.

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OTA2

Theoretical study of temperature dependent behaviour of crystal phases in $SrZrS_3$

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Abstract

Chalcogenide perovskites have been identified as a promising alternative to intensely studied organo- halide perovskites, but with significantly better thermal and chemical stability [1, 2]. Herein, we perform a systematic study of thermal behaviour of different phases of $SrZrS_3$, namely, distorted perovskite and the needle-like crystal phase (as shown in Fig.1) in the temperature range (0-1500 K). Using quasi-harmonic approximation (QHA) and ab-initio molecular dynamics (AIMD) based on periodic density functional theory implemented in VASP [3], we determine temperature dependent properties such as free energy change and the effects of temperature on the structural parameters for a broader understanding. Our results clearly demonstrate that QHA fails to capture significant thermal effects on the phases at high temperatures and it is necessary to implement accurate methods like AIMD. Based on our results, we also predict that $SrZrS_3$ exhibits a first- order phase transition from needle to DP at $\sim$ 1100 K and a quasi-second-order phase transition from orthorhombic to quasi-cubic DP at $\sim$ 1500 K.

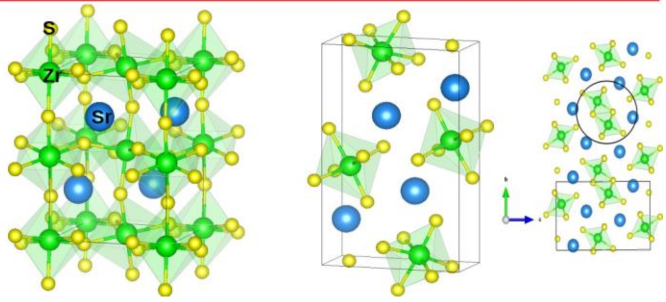

Figure 1: Crystal structure: Distorted perovskite (left), Needle perovskite (right)

Formation of a suspended magnetic layer between graphene layers through fluorine intercalation

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Abstract

Atomic spins are hard to stabilize in a condensed system while diatomic molecules in their ground state are hardly spin-polarized. By intercalating fluorine molecules between two graphene layers, here we proposed a middle path, where the molecules are pseudoatomized through bond stretching leading to stabilization of spin-polarized ground state with long-range magnetic ordering. The density functional calculations and molecular dynamics simulations show that the stretched fluorine dimers form an artificial layered van der Waal Heterostructures. The intercalated layer stabilizes in dimerized triplet and doublet states with the aid of charge transfer from the carbon atoms while the host retains its pristine band structure. The idea of pseudoatomization through intercalation can be expanded to other layered and 2D materials to form a new class of mesoscopic spin systems which in turn will serve as a platform for generating exotic quantum states and for wider application in quantum electronic devices.

OTA4

Enhanced Hydrogen Evolution Activity at the Edges of $MPSe_3$ (M=Mn, Fe) Tri-chalcogenide Layers

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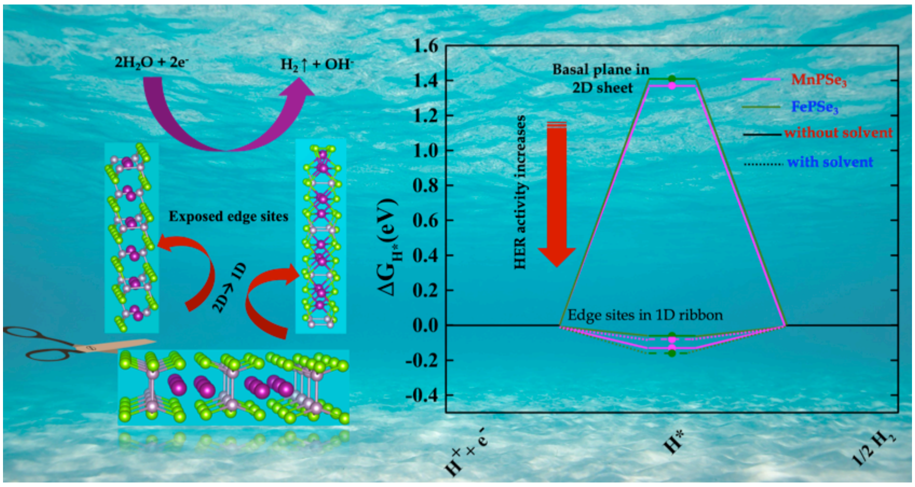
In this work we have investigated the hydrogen evolution reaction (HER) catalytic activity of two $MPSe_3$ (M: Mn, Fe) nano-ribbons with selected edge sites using first-principles density functional theory (DFT) based electronic structure calculations. Both these materials belong to the layered metal phosphite tri-chalcogenides family. In a very recent experiment[1], Gusmão et al. studied the HER activity of a series of these $MPSe_3$ bulk compounds among which $FePSe_3$, followed by $MnPSe_3$ showed the best efficiency, next to Pt (the best known HER catalyst till date), among their considered systems. On the other hand, in our earlier work,[2] we screened a large number of ternary transition metal tri-chalcogenide monolayers to study their hydrogen evolution activity on the corresponding basal planes, through determination of the hydrogen adsorption free energy (ΔG_{H*}). At the end of our screening we found that both $FePSe_3$ and $MnPSe_3$ have quite large ΔG_{H*} values indicating that these are not at all good catalysts for HER. This apparent discrepancy may have been caused by the fact that we adsorbed hydrogen only on the basal plane. There are materials (e.g. MoS_2 monolayer) where the basal planes are not active but the edge sites show efficient catalytic activity. This could be the case in our systems also. Therefore, to resolve this discrepancy, and to have a deeper understanding, we have studied catalytic activity of the edge sites of single layers of these materials.[3]



Different edges are exposed by constructing several nanoribbons from the corresponding monolayer. Thereafter, the stable most ribbon structures are considered for further investigation of their HER activity. The HER catalytic activity has been predicted through determination of the $\Delta G_{\mathrm{H}*}$ both with and without solvation effect. During this activity prediction, we have also explored the hydrogen coverage dependency. Based on Nørskov's approach of reaction coordinate mapping, we have envisaged the HER active edges for these two compounds while successfully addressing the correspondence between the experimental observation and theoretical prediction. From our DFT calculations it has been observed that the free energy of hydrogen adsorbed on the edge sites are much lower from our previously calculated values suggesting the edges as catalytically active regions in these materials.

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Rashba Band Splitting in Methylammonium Lead Iodide: An Insight from Spin-Polarized Scanning Tunneling Spectroscopy

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A low recombination rate of photogenerated carriers in methylammonium lead iodide ($MAPbI_3$) enhancing the carrier lifetime and thereby diffusion length is believed to be occurred due to Rashba band splitting [1] which arises due to a large spin-orbit coupling (SOC) arising out of high-*Z* elements (lead and iodine) in the compound along with a lack of centrosymmetry which appears due to a tilted PbI_6 octahedra and rotating electric dipoles of the organic ions leading to an effective magnetic field and thereby lifting the Kramer's spin-degeneracy of the electrons.[2] Regarding the spin-rotation or spin-texture (χ) of the two split-levels, two schools of thought persist amongst theoreticians: (1) spin-forbidden transition model and (2) spin-allowed transition model. In the spin-forbidden transition model, after spin-split, the CB and VB closer to the Fermi energy possess opposite spin-textures. A recombination between electrons in CB-minimum and holes in VB-maximum is hence a spin-forbidden process leading to a low recombination rate and thereby an enhanced carrier lifetime and a longer diffusion length.[1] On the other hand, such possibility has been overruled in the spin-allowed transition model as CB and VB possess a similar type of spin-texture closer to the Fermi energy where the recombination of photo-excited carriers is apparently possible due to spin-allowed nature of the transition.[3] In this regard, we have reported an experimental observation of Rashba splitting in $MAPbI_3$ through spin-polarized scanning tunneling spectroscopy to probe the split bands.[4] dI/dV spectra recorded at many different points of the film allowed us to spot both the Rashba split-levels and also to deliberate on their spin-textures. We observe that the bands split in such a manner that the conduction and valence bands closer to the Fermi energy have the same type of spin-textures (a spin-allowed transition model). Still a low recombination rate of photogenerated carriers in $MAPbI_3$ has been envisaged by considering Wannier-type excitons, a molecular nature of spin-domains as observed from the dI/dV images, and therefore a spin-forbidden nature of inter-domain transition.

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Hysteresis study in salt-assisted CVD grown monolayer MoS_2 field-effect transistor by pulsed I~V technique

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Atomically thin monolayer MoS_2 is manifested to be a versatile 2D material owing to its prevalent applications in future low power electronics. Overcoming certain limitations of CMOS devices using silicon-based technology, monolayer MoS_2 based FETs are leaving their signature marks for their high field-effect mobility values and current ON/OFF ratios at room temperature. Despite being a potential candidate for thin-film transistors, some of its electrical performances are merely affected due to the hysteresis and inevitable charge trapping phenomena. The exploration of the underlying mechanisms behind these hysteretic behaviors is essential for the enhancement of the carrier mobilities. In this work, we discuss a comprehensive approach towards the reduction of hysteresis in the case of salt-assisted CVD-grown monolayer MoS_2 field-effect transistor. By using the Quantum Espresso software package, DFT calculations are employed to study the interfacial properties between drain/source electrode (Ag) and monolayer MoS_2 as a channel material for FET. Based on the projected band structure calculations, the Schottky barrier is calculated to be 153 meV indicating the formation of a smoother interface between Ag and monolayer MoS_2 for high carrier transport. As the DC measurement has its limitations on evaluating the hysteresis study due to a comparatively longer period measurement process causing high gate-bias stress effects, we switch to an alternative method of using pulse I~V technique to further characterize the transistor. By employing an ultra-short pulse I~V amplitude sweep methodology, we reveal a significant reduction of hysteresis in transfer curves along with a 100% increase in field-effect mobility as compared to DC mobility values as shown in the figure. To correlate these results, we perform a single pulse time-domain drain current measurements to unleash the fast and slow transient

charge trapping phenomena. Our approach might be useful in studying the hysteretic behaviors in other 2D materials and controlling these fundamental properties may open a new dimension in future multi-bit memory, logic, and sensor-based devices.

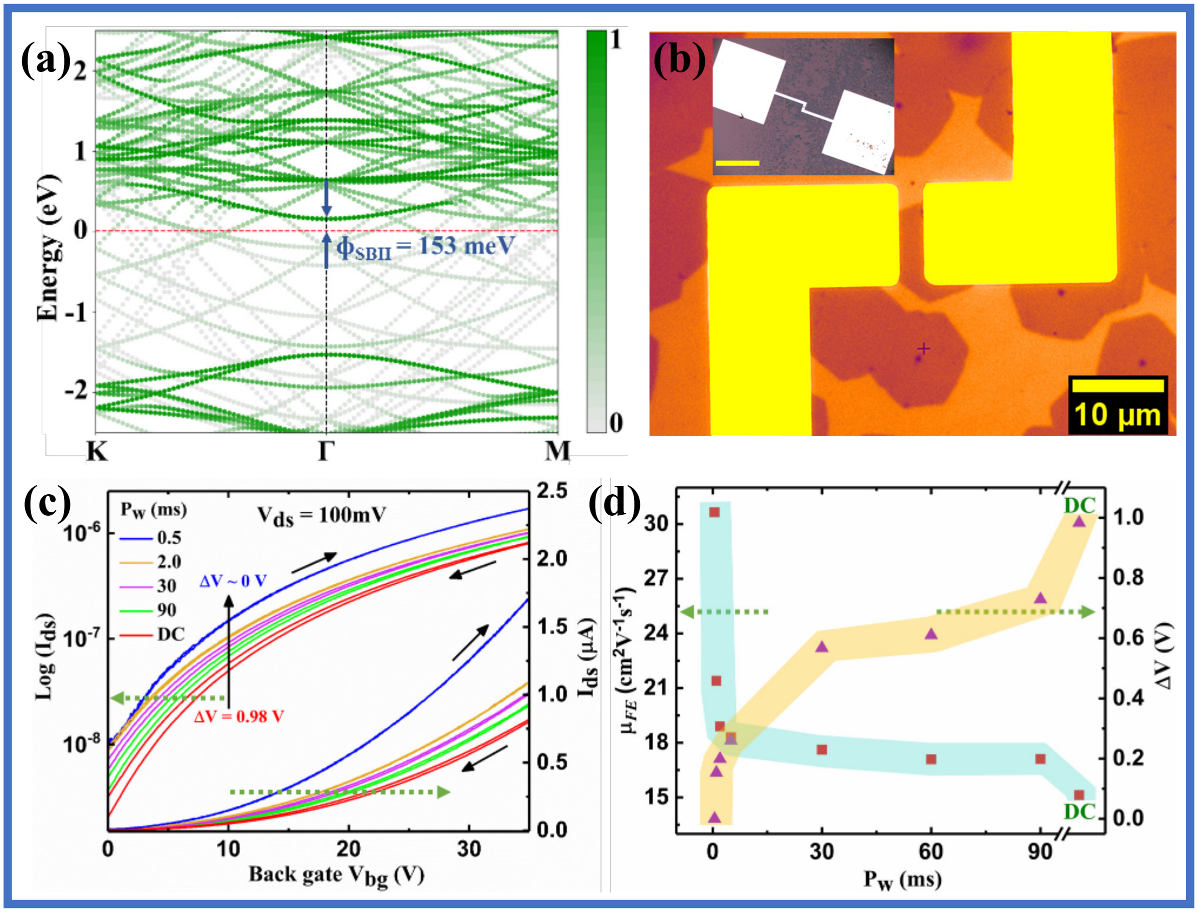

Figure 1. ***(a)*** *Projected band profile of MoS_2/Ag (111) heterostructure showing the projection of MoS_2 bands (dotted green lines) with scalebar, The n-type Schottky barrier height (Φ_{SBH}) is shown in blue color.* ***(b)*** *An optical microscopic image showing as-fabricated monolayer MoS_2 FET (Ag electrode is shown in false yellow color), Inset shows the low magnification image of the device with Ag contact pads (scale bar is 200μm).* ***(c)*** *Pulsed I~V characterization with short-pulse amplitude dual-sweeping technique for base voltage fixed at 0V. Pulse amplitude is swept monotonically at a step of 0.1V to the highest amplitude of 35V at a fixed DC bias of V_{ds} = 100 mV. The transfer curves are obtained for gate voltage pulse widths, P_w = 90, 30, 2, 0.5 ms, and corresponding drain currents are shown in both semi-logarithmic (left axis) and linear (right axis) scales. A DC transfer characteristic is shown with the same sweeping rate and dual-sweeping range for the comparison. The vertical black arrow indicates a decrease in hysteresis widths (ΔV) from DC to pulse currents with decreasing pulse widths.* ***(d)*** *Variation of mobility (left axis) and hysteresis width (right axis) with different pulse widths, P_w, and comparison with DC mobility.*

Topological Fermi-arcs and Weyl node connectivity in ferromagnetic Weyl semimetal Co3Sn2S2

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Denmark Microsoft Quantum – Copenhagen, Denmark

Abstract

Existence of topological "Fermi-arc" surface states is guaranteed by the bulk Weyl nodes and appears as a consequence of bulk-boundary correspondence in Weyl semimetals. Bulk Weyl nodes are formed when nondegenerate band touches each other under broken inversion or time reversal symmetry. We carried out scanning tunneling spectroscopy experiments on three distinct surface terminations of the ferromagnetic semimetal $Co_3Sn_2S_2$ to verify its classification as a time reversal symmetry broken Weyl semimetal [1]. We extensively visualize the topological Fermi-arcs surface states on each surface terminations. We further show that the distinct surface potential imposed by the three different surface terminations lead to the modification of the Fermi – arc contour and Weyl node connectivity. On Sn surface, we identify Weyl node connectivity of Fermi – arcs within the Brillouin zone where on Co termination the connectivity is across the adjacent Brillouin zones. On the S termination the Fermi – arcs hybridize with the non-topological bulk and surface states which hinder the exact identification of the Weyl node connectivity.

1. Fermi-arc diversity on surface terminations of the magnetic Weyl semimetal $Co_3Sn_2S_2$ Noam Morali*, **Rajib Batabyal***, Pranab Kumar Nag*, Enke Liu, Qiunan Xu, Yan Sun, Binghai Yan, Claudia Felser, Nurit Avraham, Haim Beidenkopf, *Science* **365**, 1286 (2019). (* equal contributions)

Note: This work was done at *Weizmann Institute of Science*.

OEX4

Unveiling the role of V-V dimerization on insulator-metal transition and optical transmittance of VO_2 thin films

Vanadium dioxide (VO_2) is known to undergo first order insulator to metal transition (IMT) around 341 K. IMT in the VO_2, accompanied by a structural transition from the insulating monoclinic, M1 ($P2_1/c$) structure to metallic rutile, R ($P4_2/mnm$) structure. The structural transition in VO_2 from the rutile to the monoclinic structure transforms the equally spaced V atoms, oriented along the rutile c axis, into paired (dimerized) and tilted V atoms in the monoclinic structure. VO_2 also undergoes dramatic modification in optical properties like switching in transmittance/reflectance of the IR radiations with the insulating phase being transparent to the IR while the metallic phase blocks them. This property of VO_2 is potentially useful for designing the energy saving thermochromic windows.

We have studied effect of the electron-doped ions tungsten (W^{6+}) and the hole-doped ions terbium (Tb^{3+}) ions on the IMT and optical transmittance properties of VO_2. Electron dopant W atoms are found to significantly reduce the IMT temperature in the VO_2 thin film by stabilizing the rutile metallic phase, contrary to the hole dopant Tb atoms which favor and stabilize the insulating monoclinic phase. Loss of the V-V dimerization is clearly observed due to the W doping while the Tb doping is found to strengthen the V-V dimerization. Loss of the V-V dimerization has been found to directly influence the spectral weight of the V $3d_{||}$ states, a decrease and an increase in spectral weight of the V $3d_{||}$ states has been observed due to the W and the Tb doping, respectively. Changes in strength of the IMT, the electrical conductivity, the IR switching temperature, and the solar modulation ability due to the W and Tb doping are found directly related to the spectral changes in the $3d_{||}$ states.

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Abstracts

POSTER Presentations
Theory Development (PTD)
Theory Application (PTA)
Experiment (PEX)

Semi-local DFT Advancement on Full Potential Localized Basis Scheme for Semiconductor Band-gap Prediction and Beyond

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ABSTRACT

Even in this era of computational advancement, the density functional theory (DFT) of semiconductors is still an open challenge. The absence of exact definition of exchange- correlation (xc) functional bound us to approximate. The analytical xc functional within the semi-local regime, i.e, local density approximation (LDA), and generalized gradient approximations (GGA), as well as advanced meta-GGAs are still short of finding the solution of the band-gap riddle. However, semi-empirical corrections are time-proven to be an efficient alternative. Even, in the plethora of semi-empirical xc functionals within GGA or meta-GGA group, only few are successful till date **[1]**. The key of success is the exact reproduction of the asymptotic nature of the exchange potential **[2]**. However, the choice of basis function also plays a pivotal role in the performance of DFT approximations. The combination of localized basis set of Full Potential N-th order Muffin Tin Orbital (FP- NMTO) **[3]** and the vanLeeuwen and Baerends (vLB) corrected LDA **[4]** is proved to be a perfect companion in reproducing the asymptotic potential. The success reflects on the almost exact estimation of the structural and electronic properties of group IV and III-V semiconductors **[5]** and its role in finding out a better alternative for photocatalysis among C_3N_4 polymorphs exhibits its applicability in modern-day research **[6]**. Possessing a localized basis makes the extraction of tight-binding (TB) parameters from vLB-FP-NMTO straight- forward and those TB parameters can lead the theoretical investigation on random alloys and many other interesting systems.

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PTD2

Manipulation of Magnon Modes in alloy

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ABSTRACT

The power of real-time TDDFT is demonstrated by simulating multiple magnon modes in multi-sublattice alloys, where these modes can be visualized in real space and their response to external pulses can be investigated in real-time. The results in the case of two magnetic sublattice alloy suggests the existence of element specific decoupled magnon modes along with the coupled modes. These decoupled modes indicate that the constituent elements in the alloy respond at different timescales. Using these studies three distinct ways of ultrafast laser pulse control of magnon modes is demonstrated: (1) element selective destruction of magnon modes, (2) creation of a transient non-collinear state by destruction of specific magnon modes, (3) renormalization of the optical magnon frequency, where we found a linear dependence between the laser intensity and the decrease of the magnon frequency

Two-dimensional (2D) Transition metal chalcogenides (TcX_2, X=S, Se) for charge transport in Perovskite Solar Cells: A DFT exploration

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Abstract

Exploring two-dimensional (2D) materials for using as charge transport materials in Perovskite Solar Cells (PSCs) is emphasized in this study with Density Functional Theory (DFT) analysis as a study tool. Simple and layered crystal structures of inorganic, transition metal di-chalcogenides (TcS_2, $TcSe_2$) are considered for this work. The band edges alignment of these materials with respect to the perovskite ($MAPbI_3$) band positions, is studied for the material to use as either ETL or HTL. Conventional DFT with more accurate hybrid functionals (HSE06) is used in the VASP code for this scrutiny. Band gap and the band edge dependency on 2D layer increase is also explored. We have re-established the band edge positions of TcS_2, and $TcSe_2$ and found that they can be suitable for electron transport in PSCs. Further a study on Bader charge analysis between perovskite-(TcS_2, $TcSe_2$) was conducted.

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PTA2

Unusual magnetic and electronic properties of Al-substituted Ga_2MnNi: An ab initio study

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Abstract

In the recent years searching for new Heusler alloys with novel electronic and magnetic properties have become a fascinating topic of interest to the researchers, from the point of view of fundamental understanding as well as its possible practical applications as ferromagnetic shape memory alloy (FSMA). Using density functional theory (DFT) based calculations, we have studied the effect of the replacement of the Ga atoms by the Al atoms in the alloy Ga_2MnNi and have predicted a new energetically stable Heusler alloy Al_2MnNi. By analyzing the magnetic properties, we find that Al_2MnNi alloy possesses a substantially lower value of magnetic moment compared to Ga_2MnNi, despite the presence of Mn atom in the system. To understand this unusual result of near-quenching of Mn moment (Figure 1a), we have calculated and analyzed atom-projected spin-polarized density of states (DOS) for the $Ga_{2-x}Al_xMnNi$ systems. These results suggest that a shift of peak position in the minority DOS for the Mn atom to the occupied region in Al_2MnNi, as compared to Ga_2MnNi, leads to the decrement of moments of the Mn atoms in Al_2MnNi. Further, analysis of the difference charge density distribution shows that Mn atoms have more localized charges around them in Al_2MnNi as compared to Ga_2MnNi, which also corroborate with the Bader charge analyisis, where we found that Mn atom in Al_2MnNi has gained an appreciable amount of charge, which was lost by the Al atoms. To understand the Mn-Mn exchange interactions, the Heisenberg exchange coupling parameters (J_{ij}) between the Mn atoms, as a function of distance between them, have also been probed. We found that the Mn-Mn exchange interaction is to be of indirect RKKY-type. Interestingly, in Al_2MnNi we find a relatively large DOS near the Fermi energy. Hence, electronic properties of such system with partial substitution of 50% Ni atoms by Co atoms at the C-site of Al_2MnNi have been explored. Combined results of calculations of Bloch spectral functions and DOS of this material suggest an interesting possibility of existence of a feature like van Hove singularity in the density of states very close to the Fermi level in the $Al_2MnNi_{0.5}Co_{0.5}$ system (Figure 1b).

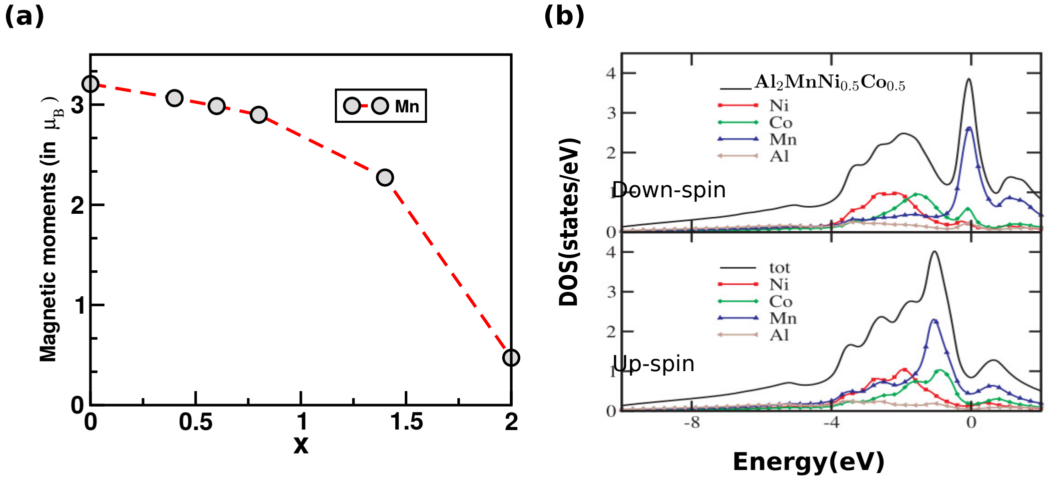

Figure 1: (a) Magnetic moment of the Mn atom for $Ga_{2-x}Al_xMnNi$ as x is increased from 0 to 2 ; (b) Spin-polarized partial density of states of all the atoms in $Al_2MnNi_{0.5}Co_{0.5}$ system.

Electronic properties and microscopic modeling of Polymeric Fe(II) triazole

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Abstract

In spin crossover materials, an abrupt phase transition between a low-spin state and a high-spin (HS) state can be driven by temperature, pressure or by light irradiation. Of special relevance are Fe(II) based coordination polymers where, in contrast to molecular systems, the phase transition between a spin $S = 0$ and 2 state shows a pronounced hysteresis which is desirable for technical applications. A satisfactory microscopic explanation of this large cooperative phenomenon has been sought for a long time. The lack of x-ray data has been one of the reasons for the absence of microscopic studies. In this work, we present an efficient route to prepare reliable model structures and within an *ab initio* density functional theory analysis and effective model considerations we show that in polymeric spin crossover compounds magnetic exchange between HS Fe(II) centers is as important as elastic couplings for understanding the phase transition. We discuss the relevance of these interactions for the cooperative behavior in these materials.

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Functionalization of monolayer MoS_2 by applying mechanical strain

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Abstract

Two-dimensional (2D) transition metal dichalcogenide MoS_2, with its intriguing physical and chemical properties, is emerging as a promising material for various future applications. MoS_2, an indirect band gap semiconductor in its bulk form, becomes a direct band gap semiconductor in the monolayer limit with a band gap that falls within the visible range. Tunability of the band gap of monolayer MoS_2 can be extremely useful for applications in future optical and electronic nanodevices. Strain engineering has proved to be an efficient way to tune the band gap. From our first principle density functional theory (DFT) based calculations it is seen that monolayer MoS_2 is extremely sensitive to the application of in- plane uniaxial and biaxial strain. With the application of different types of strains, it is observed that the mechanical strain not only influences the magnitude of the band gap and the electronic structure, but also causes the direct to indirect band gap and the semiconductor to metallic transition. From the analysis of the electronic structure, it is observed that the driving force behind the transitions is the changes in the strength of interaction between the Mo-*d* and the S-*p* orbitals due to the changes in the bond lengths and the bond angles upon application of strain. Thus, by considering the various strain profiles, our calculation substantially provides a pathway to the engineering of the electronic and optical properties of MoS_2.

In order to make MoS_2 and other two-dimensional nanomaterials suitable for the development of low-dimensional spintronic devices, different approaches are required to effectively induce and manipulate the magnetism, as the pristine monolayer of MoS_2 is intrinsically nonmagnetic. It is known that the defects due to atomic vacancy, such as single Mo vacancy and single or double S vacancy are particularly common in MoS_2 monolayers grown by chemical vapour deposition (CVD) method. CVD happens to be the most convenient way for the production of large area monolayer films. Vacancy defects can be easily and controllably obtained in CVD growth process or even using the electron beam irradiation of MoS_2 films. In our DFT calculations, it is observed that the vacancies produce in-gap states within the band gap of monolayer MoS_2, but cannot induce magnetism. Upon the application of in-plane biaxial tensile strain in these vacancy doped systems, the band gap closes with the simultaneous appearance of a significantly large spontaneous magnetic moment in all the three cases, unlike the pristine MoS_2, which remains nonmagnetic. The critical strain (~ 9-10%) required to induce magnetism is well below the breaking limit of these systems. Such a strain-induced magnetism in these systems can be understood from the itinerant origin based on the analysis of the electronic structures and the charge density at the critical strain. The delocalized electrons around the vacancy sites are believed to be responsible for the emergence of such magnetism in the defect doped MoS_2. Although the experimental results on this phenomenon are not yet available, this result may provide an opportunity to develop new types of spintronic devices based on two-dimensional materials.

Probing the martensite transition and thermoelectric properties of Co_xTaZ (Z = Si, Ge, Sn and x = 1, 2): a study based on density functional theory

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Abstract:

In the last few decades, there has been a tremendous increase in the research on Heusler alloys, due to the importance and relevance of these materials, both from the points of view of application as well as fundamental understanding. These alloys exhibit different exotic properties like, shape memory effect, thermoelectric and spintronic properties etc. In this work, using density functional theory based electronic structure calculations, we carry out a comparative study of geometric, mechanical, electronic, magnetic, and thermoelectric properties of CoxTaZ alloys, where Z = Si, Ge and Sn and x = 1 and 2. A systematic approach has been taken to perform calculations first to probe the possibility of existence of a tetragonal (martensite) phase in these alloys and then to perform a comparative study of various physical properties of the six systems, mentioned above, in the cubic and possible tetragonal phases. From our calculations, a tetragonal phase has been found to be stable up to about 400 K in case of Co_2TaSi and Co_2TaGe alloys, and up to about 115 K for Co_2TaSn, indicating the presence of room temperature cubic phase in the latter alloy, unlike the former two. Further, the results based on the energetics and electronic properties have been found to corroborate well with the elastic properties. All the above-mentioned full Heusler alloys (FHAs) show magnetic behavior with metallicity in both the phases. However, their half Heusler counterparts exhibit non- magnetic semi-conducting behavior in the cubic phase. Further, we calculate and compare the thermoelectric properties of all the materials in the cubic and possible tetragonal phases. In the cubic phase, the half Heusler alloys exhibit improved thermoelectric properties compared to the respective FHAs. Furthermore, it is observed that the FHAs exhibit higher (by about an order of magnitude) values of Seebeck coefficients in their cubic phases, compared to those in the tetragonal phases (which are of the order of only a few micro-volts/Kelvin). These results have been understood from the transport properties as well as the band structure and topology of the Fermi surface of the probed materials.

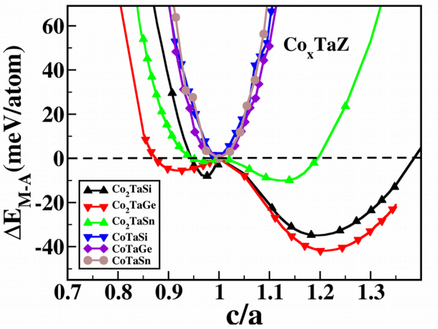

FIG. 1: Plot of variation of energy difference between the tetragonal (M) and cubic (A) phase(ΔE_{M-A}) in Co_xTaZ (Z = Si, Ge and Sn), x = 1, 2 with respect to c/a

Electronic and topological properties of strain induced transition metal trichalcogenides

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Abstract

Weyl semimetals are conductors whose low-energy bulk excitations are Weyl fermions, and the surfaces have metallic Fermi arc surface states. These Fermi arc surface states are protected by a topological invariant related with the bulk electronic wave functions of the material. In the present work, we study the electronic band structure of transition metal trichalcogenides HfS_3 and ZrS_3 having structure $P2_1/m$ with and without strain by density functional theory (DFT) incorporating the generalized gradient approximation (GGA) of Perdew-Burke-Ernzerhof (GGA- PBE). The electronic band structure of transition metal trichalcogenides with strain was calculated and a band crossing between valence band and conduction band along X - Γ - Z direction was observed. Afterwards the topological properties of strain induced transition metal trichalcogenides were also studied by using Wannier90 function, implemented in Wannier90 and Wannier Tool code. Our study proves that the strain induced transition metal trichalcogenides are topological semi-metals.

Strain-engineering-based study of 2D Multiferroic $VOCl_2$ Monolayer

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Abstract

Two-dimensional (2D) magnetoelectric multiferroic materials are a special class of 2D materials that holds promising applications in the miniaturization of logic and memory devices, along with the possibility to realize new low-dimensional device architectures. In this work, for the first time, we have reported a strain-engineering- based study for a 2D multiferroic material, $VOCl_2$ monolayer, that shows independent control of magnetic and ferroelectric properties via applying strain along the different in-plane crystallographic directions. An in-plane strain of around 4% along the non-polar axis was found to cause a transition from an antiferromagnetic (AFM) ground state with an out-of-plane magnetization to a ferromagnetic (FM) ground state with in-plane magnetization. Additionally, the tensile strain along the polar axis enhances the ferroelectric polarization. An increase in the ferroelectric switching energy barriers and the magnitude of the magnetic exchange coupling parameter suggest enhancing ferroelectric and ferromagnetic stability with tensile strain. The work reveals the $VOCl_2$ monolayer as a strain- tuneable multiferroic material holding great promises for future generation nanoelectronic devices.

Calculation of Quantum Capacitance and Pseudo-capacitance of Ti,Nb,Mo,V based Pristine and O-functionalized MXene using Density Functional Theory

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Abstract

Supercapacitors' (SC) concept has revolutionized advances in energy storage and applications due to their power densities greater than those of batteries and energy densities higher than conventional capacitors. Electrical Double Layer Capacitor(EDLC) and Pseudo-capacitor(PC) are the two types of SCs that follow non-Faradaic and Faradaic charge storage mechanisms. The performance of a supercapacitor depends on the electrode material and the electrolyte. The available surface area of the electrode materials turns out to be very important for supercapacitor performances. The electrode material's total capacitance results from the electrode material's quantum capacitance, pseudo-capacitance, and EDLC under working conditions. The EDLC and material's quantum capacitance is in series combination, and the pseudo-capacitance is in parallel combination with them.

Recently discovered two-dimensional(2D) transition metal carbides (nomenclature as MXenes) have shown remarkable performance as negative electrodes for SCs. In this work, using the Rigid Band scheme, we calculate the Pseudo-capacitance and Quantum capacitance of Ti, Nb, Mo, and V based pristine and functionalized MXene theoretically.

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Effect of Mn on the precipitation kinetics of Al-Cu alloy

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Abstract

Aluminum alloys are attractive in aviation, aerospace and automobile industries because of their high specific strength [1]. Conventionally, Mn is used in 2xxx series Al-Cu alloys to modify the morphology of detrimental Fe-rich precipitates formed during casting and solidification [2, 3]. Recent studies, however, have shown that Mn can stabilize metastable θ' precipitates in these alloys through preferential segregation at the semi-coherent interface between the precipitates and the matrix, which enables the Al-Cu alloys to sustain strength at higher temperatures [4, 5]. In the present study, we have prepared Al-Cu-Mn alloys with varying amount of Mn (0.3-0.8 %wt.) and investigated the formation of nanoscale precipitates and their role on alloy strength. It is observed that for high Mn content, (0.8%wt.) formation of twin containing *T*-phase precipitates was accelerated and the formation of θ' precipitate was suppressed. This trend of precipitate formation is reversed in low Mn containing alloys. The former alloy thereafter provides a better room temperature mechanical response (hardness) compared to the later one.

First-principles density-functional-theory calculations reveal that the interfacial energy of *T*- phase precipitates with the Al matrix is comparatively higher than that of θ' precipitates, which is one of the key factors governing nanostructure evolution with varying Mn addition. We also find that the segregation energy of Mn to the Al/*T*-phase interface is lower than that of Al/ θ' interface, In future course, we plan to investigate other factors such as elastic misfit strain energy on alloy-precipitate interfaces.

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Understanding the Stability of Edge States in SiC Nanoribbons by First Principles Approach

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Abstract

Understanding the edge states in 1-D nanostructures plays a crucial role, as it helps to design and develop the quantum mechanics-based nano-devices [1,2]. Similar to graphene and silicene, the structural stability of atomically thin SiC nanosheet, feasible synthesis mechanism and the electronic properties were reported [3]. The monolayer SiC was shown to be direct band gap, whereas, bilayer and bulk SiC are indirect wide band gap semiconductors. Utilizing these advantages of atomically thin-monolayered nanosheet, the structural stability and electronic properties of edge states are studied, in the present work, by employing first principles density functional theory calculations. For this work, various widths of both arm-chair and *zig-zag* SiC nanoribbons as well as hydrogen passivated ribbons are also considered. Our calculations show that the structural stability of *zig-zag* SiC nanoribbon is higher when compared to arm-chair case. In addition, arm-chair SiC nanoribbon is electronically insulative, while the *zig-zag* nanoribbons are having half-metallic nature and also, possessing the spin polarized edge states. The stability and growth of edge states in SiC nanoribbon are also explored by introducing the mechanical strain and chemical substituents.

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PTA11

AB-INITIO MOLECULAR DYNAMICS STUDY OF CESIATED MOLYBDENUM SURFACES

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Abstract

Cesiated molybdenum surface serves as a construction material for the present generation of negative hydrogen ion sources that are being developed for the needs of the nuclear fusion research [1]. The cesium is introduced in order to reduce the work functoin (φ) of Mo, which increase the effeciency of the electron extraction [2]. Ab-initio molecular dynamics calculations based on DFT as implumented in VASP [3] have been employed to investigate the finite temperature structure of clean Cs surfaces and cesiated Mo(001) and the effect of T on the work function. The Cs atoms in all but the first adsorption layers will experience relatively weak interactions with the Mo atoms and hence the cohesion of these layers will be largely determined by the Cs-Cs interactions. Therefore, one can expect that the behavoir of Cs atoms that are not in a direct contact with Mo will be very different from that of the atoms from the first layer. Firstly, we will consider clean Cs(001) and Cs(110) surfaces representing exterme cases of systems, where the interaction with the Mo is negligible. Two different simulation temperatures have been considered:T_1= 223 K is below and T_2= 423 K is above the melting temperature of Cs and corresponds to the typical operating temperature in the H^- sources. The thermally induced structural changes occuring mainly in the three free layers contribute to a significante variation of work function. At T_1, the surface layers exhibits a bulk-like behavior and the work function values of Cs(001) and Cs(110) are close to their zero T values. Upon increasing the temperature to T_2, the two topmost layers of Cs (001) and Cs(110) are transformed to a disordered phase and both work function values converge to same value. Secondly, high temperature simulations are executed for the Cs deposited on Mo(001) with multilayer depo- sition. Our results show that the stucture of Cs/Mo(001) shares similarities with that of Cs(001) and Cs(110). Thus the computed φ of Cs+Mo(001) is similar to that for Cs surfaces.

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Transition metal implanted oxide as support for noble metal single atoms

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Abstract

Using first-principles modelling based on density functional theory (DFT) we show that transition metal (TM) atoms if implanted, can be stabilized as interstitial in rock- salt structured oxides depending on their ionic radii and oxygen affinity. Based on defect formation energy, transition barrier and diffusion coefficient calculations from DFT we show that it is possible to predict whether a TM dopant will be stable in an oxide or will precipitate out. Following that we also show that oxides such as BaO with TM implanted as interstitial can be used as an efficient support for noble metal single atoms (SAs). We use this finding to solve a long standing challenge in the field of heterogeneous catalyst: stabilizing noble metal single atom catalysts. As single atoms are highly mobile in nature and are prone to agglomeration it is very difficult to stabilize them. We show that TM-implanted BaO not only binds the single atoms strongly but also resist cluster formation and hence can serve as an ideal support for the SAs. Interstitial doping of TMs for stabilizing SAs is beneficial over substitutional doping of TM in oxides as interstitial doping provides the maximum utilization of the dopant and can bind more SAs. Finally we attribute the strong binding of the noble metal SAs and prohibition of cluster formation on TM-doped BaO to the charge transfer from the TM dopant to single atoms.

PTA13

Thermodynamics of Hydrogen Evolution from Surfaces of Earth-abundant Cu_2BaSnS_4

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Abstract

Cu_2BaSnS_4 (CBTS) has recently emerged as a promising candidate for low-cost solar light conversion devices. This semiconductor possesses highly desirable qualities like direct bandgap (~1.8 eV), high carrier mobility, environmentally benign composition, solution-processibility, and absence of deep defect states. Just a few years back, CBTS was fabricated in thin-film and nanocrystalline form and soon after, multiple experimental studies have shown good photovoltaics and solar-to-hydrogen conversion efficiencies arising from CBTS and its' Selenium alloyed counterparts. However, till now no effort has been spent on growing selective facets of this material for photocathodes. Selective growth of preferred surfaces has historically resulted in drastic improvement of catalytic activity of electrocatalysts like MoS_2, Pt etc. In order to fill this gap, by using Density Functional Theory, we investigated the electronic structures and the mechanism of Hydrogen evolution of five probable low-indexed surfaces of CBTS. Among the studied surfaces, we find the Ba-rich (001) to have the most suitable thermodynamics for the hydrogen conversion reaction where the H_2 formation follows Volmer-Heyrovsky mechanism. Further, we found that alloying Selenium on the surface of CBTS, makes the thermodynamics even more favourable. Our results will help to improve the photocatalytic hydrogen conversion efficiency by selectively growing preferential facets for Cu_2BaSnS_4 photocathodes.

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PTA14

XANES simulations in diamond-like two-dimensional materials

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Abstract

In 2004 a new era on the searching of better-performance materials had given its jumpstart with the emergence of the thinnest material ever synthesized[1]: the well-known graphene. Since then, many atomic- sized materials have been obtained from layered bulk materials and successfully characterized by many methods, including x-ray absorption spectroscopy (XAS). A few years ago, such a technique was employed to study bulk diamond-like materials, as well as graphite, in order to better characterize this sp^2/sp^3 bonded materials[2]. Recently, researchers from Minas Gerais, Brazil, have theoretically and experimentally studied the formation and stabilization of diamondol[3], a 2D hydroxylated diamond-like layer, which arises from pressure-dependent charge injection on bi-, and multilayer graphene in a controlled ambient environment using scanning probe microscopy (SPM) along with electric force microscopy (EFM) measurements. Bearing that in mind, we have theoretically investigated sp^2 and sp^3 carbon-based materials through Density Func- tional Theory calculations and XANES (X-ray Near-Edge Spectroscopy) simulations. Diamondol, in turn, is composed by a mixture of sp^2 and sp^3 carbon bonding, and our simulations have shown that XANES may be an excelent way to characterize this kind of material.

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PTA15

Synergetic effect of localized and delocalized π electron on Li storage properties of Si/C heterostructures

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Abstract

The composition of two different categories of anode materials, i.e. layered and alloy type is the future of anode material in Li-ion batteries. In our work, using First-principles approach, we proposed multilayer heterostructure of graphene/graphite (layered type) with silicon monolayer (Si-ML) (origin is alloy type), as a potential anode material for LiB's. The synergetic effect of the delocalized π electron of carbon and localized π electron of Si-ML plays a crucial role in maintaining the electron and ion conductivity increases the stability and specific capacity with moderate open circuit voltage. The model structures proposed in this work shows high specific capacities in the range of 748 to 438 mAh-gm^{-1}. This indicates that we can tune the specific capacity using the different ratio of carbon and silicon layers. The localized π electron helps to restrict the volume expansion within 15 % for a fully lithiated model structure. The low interlayer diffusion energy of Li-ion makes all the heterostructure as a potential anode material. The proposed study will help to understand the Li storage properties of the carbon/silicon-based composite to develop the anode materials with a certain approach.

Keywords: Batteries, Storage, Carbon, Electronic Structure, Diffusion, DFT

PTA16

DFT Investigations Into Efficient Bifunctional Catalytic activity Of Cobalt Nanoparticle Dispersed Nitrogen-Doped Graphitic Nanospheres In Rechargeable Zinc-Air Battery

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Abstract

The zinc-air battery (ZAB) is an emerging rechargeable energy storage system having high energy density with safe operation and low operation cost. Despite these advantages, the overall efficiency of these batteries is limited by the slow kinetics of the oxygen reduction and oxygen evolution reactions (ORR and OER) at the cathode (air electrode) during discharge and charge, respectively. Development of durable and efficient bifunctional catalyst is, therefore, one of the crucial challenges for rechargeable ZAB technology. Our experimental collaborators have recently demonstrated a hybrid catalyst system having cobalt (Co) nanoparticle dispersed nitrogen doped graphitic spheres (Co@NGC-NSs) as an excellent bifunctional catalytic activity toward ORR and OER in alkaline medium (Ref. 1). In order to have a microscopic picture of possible pathways for ORR and OER, and to understand why Co@NGC-NSs act as better ORR/OER catalyst, we studied these reactions on a number of model systems using first-principles density function theory (DFT) methods. We found that in the Co@NGC-NSs system, Co does not provide active sites; rather, it is the NGC surface where all the ORR and OER take place. It is also found that N doping improves ORR performance, whereas the presence of Co is responsible for the enhanced OER.

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PTA17

CO_2 capture, activation and dissociation on the Ti_2C surface and Ti_2C MXene: the role of surface structure

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Abstract

Atmospheric CO_2 is one of the main components of the greenhouse effect. To overcome this problem there are ongoing efforts to convert CO_2 to some other value added products, a strategy popularly termed as Carbon capture and utilisation (CCU). Our work focuses on converting CO_2 to CO which can then be converted to methanol, acetic acid etc. The capture, activation and dissociation of CO_2 being the preliminary steps in this process. Here we have tried to understand the role of surface composition and structure in CO_2 activation and dissociation, by studying the same on {100} surface of cubic Ti_2C and MXene, modelled for the {0001} surface of trigonal Ti_2C, with the help of first principles density functional theory based calculations. Our results show that CO_2 undergoes barrierless chemisorption on both of these surfaces involving a charge transfer from the substrate. There is a strong preference towards {100} cubic Ti_2C in terms of adsorption energy which is attributed to a lower value of the work function of the {100} surface. We also observe a correlation between the vertical/horizontal chemisorption geometry to the surface structure in these two scenarios. Furthermore, on MXene, for the different pathways considered for CO_2 dissociation, there is a barrier of 0.13 eV associated with C-O bond breaking. On {100} cubic Ti_2C however the same step requires additional energy of 0.15 eV to happen by virtue of stronger bonding of CO_2. Coverage dependent CO_2 chemisorption studies bring out the drastic changes in these substrates since on the Ti_2C surface the CO_2 molecules form clusters around the C-vacancies while on MXene they are uniformly spread on the surface. Also on MXene, CO_2 molecules are weakly attractive till 0.33 ML and then repulsive while on Ti_2C {100} the interactions are attractive upto 0.25 ML and becomes repulsive therafter.

PTA18

First Principles Study of Strain Effect on Thermal and Electrical Transport of Metal and Graphene

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bstract

The Strain effect on thermal conductivity due to phonon-electron(p-e) scattering and phonon-phonon scattering and electrical conductivity due to phonon-electron(p-e) scattering is calculated for bulk Cu,Al,Al(111),Cu(111) surfaces and graphene(Gr).We calculated the effect of both the positive strain(tensile) and negative strain(compressive) on electronic thermal conductivity(k),phonon thermal conductivity(k_p) and electrical conductivity(σ).It is found that p-e scattering plays an important role in determining the lattice thermal conductivity(k_l) of Al and Cu, while p-p scattering is dominant in case of the determination of (k_l) of semiconductor graphene.Therefore in case of metal k and in case of semi-metal k_p plays the important role in deriving k_l. Also it is found that in case of metal (Al and Cu) for both bulk and surface, with the application of negative strain till a certain range both K_l and σ increases and with the application of positive strain both k_l and σ decreases.But in case of single layer graphene with the application of both positive and negative strain it's k_l and σ decreases drastically.We also found that with the increase of electron-phonon coupling constant ( ) both k_l and σ decreases and vice versha.

Chemically Graded Metal/Ceramic Interface - A High Throughput DFT Study

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Abstract

The interface in nano-sized metal-ceramic heterostructure plays an important role in dictating their properties. Interfaces between metals and ceramics are assumed to be atomically sharp, but recent studies suggests that Ti(metal)-TiN(ceramic) system is atomically compositionally graded across the interface[1]. This chemically graded interface can potentially find applications in wear resistance coatings, barrier layer for IC interconnects, hetero-catalysts, etc. Such chemically graded interfaces have some unusual characteristics like, gradual variation of elastic modulus across the interface. Bonding at the interface could improve due to smooth variation in lattice parameter, elastic modulus and other properties. To explore other combinations of metal/ceramic systems that could plausibly result in chemically graded interface by experimental effort is formidable. Here, we performed first-principles calculations based on density functional theory to predict the formation of chemically graded interface. In Ti-TiN, chemical gradation is attributed to creation of N vacancy in TiN; and diffusion of N into interstitial site of Ti. This provides a quantitative way to calculate driving force to form a chemically graded interface. We calculate vacancy formation energy, interstitial formation energy; sum of two quantities give estimate of driving force to form chemically graded interface. We have considered different combinations of metals (M) and ceramics (M_aX_b) to evaluate if they can form a chemically graded interface, where M = Ti, Zr, Hf, V, Nb, Ta, Al, Mg, Cr, and Fe; and X = C, N, and O.

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Force Filed Parameters for Copper Proteins

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Abstract

In this study, we have derived bond-stretching and angle-bending parameters applicable to copper-containing systems which are compatible with the AMBER FF. A total of seven model systems were used to mimic the common coordination observed in the type-I, type-II, type-III, and binuclear Cu_A active sites. The Hessian matrix of each model system computed at the B3LYP/6-311++G(d,p) $\cup$ LanL2DZ level is further analyzed by Seminario's method to derive the desired force constants. The copper amber force field (CAFF) parameters for type-I, type-II, type-III, and binuclear Cu_A active sites were validated by performing molecular dynamics (MD) simulations on various copper proteins. The present study provides a comprehensive set of CAFF parameters which is consistent with the AMBER FF parameters. These parameters are also applicable to a variety of copper-containing biological systems.

Title- Electronic, half-metallic and magnetic properties of bulk Co_2TiGe heusler alloy

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Abstract

Density functional theory calculations have performed to investigate the structural, electronic and magnetic properties of bulk structure Co_2TiGe Heusler alloy. The calculation shows that Co_2TiGe is half-metallic with only two bands crossing the Fermi energy in the majority channel with total magnetic moment of $2.00\mu B$ per formula unit at the equilibrium lattice constant 5.85Å. The magnetic moments fulfil the slater-Pauling rule. From the analysis of the spin-polarized density of states, we found that the half-metallicity confirmed in bulk Co_2TiGe.

Structural, Electronic and Elastic Properties of ScP at ambient pressure

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Abstract

We investigate the structural, electronic and elastic properties of ScP phase B1 and B3. Calculations based on Density functional theory were used for the Generalized gradient approximation scheme. A semimetallic behavior is found to be seen in the B1 phase and a semiconductor behavior with a wide band gap at X is found in the B3 phase. With previous studies, our calculated results are in good agreement. To confirm the stability of these phases, we also calculate the phonon structure.

Defect induced ferromagnetism in a two dimensional metal−organic framework

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Abstract

Two dimensional ferromagnetic materials are potential candidates that can be integrated with the current nanoelectronic and spintronic device architecture. The latest trends in designing spintronic-devices are mainly based on inorganic-compounds. Here we present a study based on first-principles density functional calculations where we designed a two dimensional ferromagnetic material within the family of metal−organic frameworks. Starting from the inorganic CrI_3compound, we demonstrated a chromium based metal−organic compound i.e., $Cr(COOH)_3$. The optimized structure of $Cr(COOH)_3$is found to be thermodynamically stable. The lowest energy magnetic configuration of pure $Cr(COOH)_3$ turns out to be antiferromagnetic. Our calculations suggest that the presence of charged Cr-vacancy defects with charge i.e., 1+ and 2+ which stabilizes the ferromagnetic state over antiferromagnetic orderings. The presence of delocalized holes are found to be responsible for favoring the ferromagnetic ordering.

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First-principles study on $Cs_2MM'Cl_6$ [M= Cu, Ag, Au; M'= Al, Ga, In, Tl] double perovskite halides for Photovoltaic Applications

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ABSTRACT

A cohesive first-principles study on structural electronic and optoelectronic properties of Cs_2MM' Cl_6, M= Cu, Ag, Au and M'= Al, Ga, In, Tl] is performed. The exchange-correlation function, which is the only unknown parameter in the state-of art formulism is determined through well-known mBJ, mBJ + SOC approximation and GGA approximation. The structural optimization, tolerance factor and mechanical stability criteria confirmed the stability of the system in cubic structure symmetry. The main motive of the present work is to explore the promising materials from for high efficiency photovoltaic cell, for that the accurate measurement of band gap of a system is important. This criterion can be satisfied by using mBJ approximation with spin orbit coupling. Our computational band gap prediction using mBJ+SOC, showing $Cs_2CuAlCl_6$ and $Cs_2AuAlCl_6$ have direct band gap of value 1.40 eV and 1.51 eV, respectively. The optical properties in terms of real and imaginary part of dielectric constant (ε), refractive index (η), absorption coefficient (α), optical conductivity (σ), and reflectivity are carried out in the energy range of 0-5 eV. A stable, direct band gap with value (E_g = 1.40 eV) ideally required as well as optical parameters specially absorption and reflection spectras reflects the suitability of $Cs_2CuAlCl_6$ system for the construction of high efficiency photovoltaic cell.

PTA25

Designing multifunctional two-dimensional layered van der waals transition metal phosphorous chalcogenides

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Abstract

Layered two-dimensional (2D) transition metal phosphorous chalcogenides (TMPCs) are now in intense research focus due to their interesting ferroelectric and magnetic properties and compatibility with 2D electronic devices. Here, we have employed first-principles density functional theory calculations to investigate the electric and magnetic properties of ABP_2S_6 (A = Cu, Ni; B = Cr, Mn) TMPCs. We have systematically investigated four TMPCs compounds namely $CuCrP_2S_6$, $CuMnP_2S_6$, $NiCrP_2S_6$ and $NiMnP_2S_6$ and reported unusual anti/ferroelectric (AFE/FE) and electronic properties. We have found a more stable ferroelectric state in Van der Waals (VdW) gap with higher polarization compared to the usual ferroelectric phase in insulating state. In case of $CrMnP_2S_6$ and $NiMnP_2S_6$, we have proposed them as polar half metals. Moreover, our analysis have showed that $NiMnP_2S_6$ can undergo metal-to-insulator transition driven by the polar distortion. Finally, we have performed molecular dynamics simulations at various finite temperatures, at 300K, in case of $NiCrP_2S_6$ and $NiMnP_2S_6$ we have observed that the ferroelectric state within the VdW gap is stable. Interestingly, we have discovered a hybrid 'inter-intra' layer antiferroeletric configuration within the VdW gap for $CuCrP_2S_6$. The origin of such geometry is share strain as the layers are found to start sliding with respect to each other due to the temperature effect. The reported VdW FE/AFE states can be tuned by uniaxial strain along the perpendicular direction of the 2D layer and can be considered as potential piezoelectric materials.

PEX1

Structure, Morphology, and Photovoltaic Implications of Halide Alloying in Lead-Free $Cs_3Sb_2Cl_xI_{9-x}$ 2D-layered Perovskites

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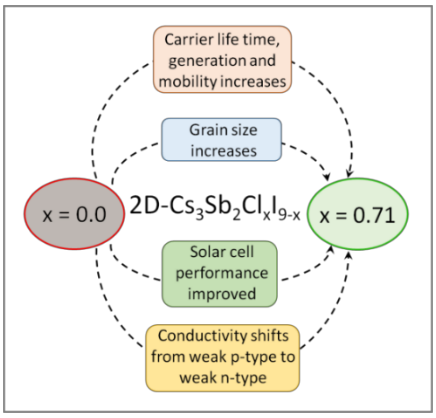
Abstract

Compositional tuning has been a major driving force behind the excellent optoelectronic properties observed in typical Pb-based perovskites. For lead-free perovskite derivatives, a challenge to understanding the connection between compositional tuning and intrinsic optoelectronic properties, hence a barrier towards boosting their performance comes from the fact that multiple crystalline substructures can form based on composition, film processing, or both. Especially with lower dimensional (0D, 1D, 2D) substructures, the particular polymorph present in the film can be a greater determinant of optoelectronic properties than the composition itself. In this work, we report a simple method to alloy the halide site in all-inorganic lead-free $Cs_3Sb_2I_9$ films while maintaining a consistent 2D-layered substructure, as a means to independently study the photovoltaic implications of halide substitution. We use a broad suite of spectroscopy and device measurements to identify an optimal stoichiometric substitution of chloride for iodide (~ 8 mol%, measured) that balances both intrinsic and bulk optoelectronic properties to achieve a top power conversion efficiency of 2.2%. This work underscores the importance of controlling substructure while investigating the impacts of compositional tuning for the development of lead-free perovskites, and more broadly validates the approach towards realizing lead-free alternative perovskite solar technologies.



PEX2

Tailoring of optical band gap and microstructure profiling of vanadium based complex compound systems

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Abstract

The oxides of vanadium have recently been acquired a great deal of consideration in diverse device applications because ofits crucial physical and chemical nature such as multi valency, band structure, tailorable optical bandgap, good chemical and thermal stability, layered structure, excellent thermoelectric property and high energy density.Herein, we report the synthesis of different combinations of complex compound system with chemical empirical formula $V_{2-x}Bi_{2x}O_{5-\delta}(0.01 \leq x \leq 0.04)$ and $V_{2-x}Mn_xO_{5-\delta}$ $(0.1 \leq x \leq 0.2)$ using high temperature solid state reaction route between the temperature range 550-650^{0}C for 48-64 hours. The structural phase purity and lattice parameters were investigated using X-ray diffraction technique. All the samples exhibit orthorhombic structure in (001) direction corresponds to that of V_2O_5. The structural parameter including grain size, micro strain, dislocation density and lattice parameters were calculated and reported here.The optical properties recorded using UV-Vis spectroscopy and photoluminescence (PL) spectra. The band gap energy calculated from Kubelka-Munk re-emission function suggests the variations from 2.16eV to 2.07eV for V-Mn-O system and 2.228eV to 2.267eV V-Bi-O for upon changes in mole fraction. The result presumed to be a significant feature for optoelectronic application. Photoluminescence spectra of the samples shows intense broad emissions with multiple excitonic emissions as wells as combined colour emissions. These PL results are indicative of suitability of materials in optical window applications preferably utilizing the thermochromic and electrochromic features.

Dynamic Response of Alternating-Current-Driven Light-Emitting Diodes Based on Hybrid Halide Perovskites

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Abstract

Hybrid halide perovskites are being considered for a wide range of applications in the domain of optoelectronic devices due to their interesting optical and electronic properties. In this work, we report the dynamic response of alternating-current-driven light-emitting diodes based on a range of hybrid halide perovskites. Electroluminescence (EL), which appears only in the positive section of a dc voltage, arises in both cycles under a sinusoidal ac voltage. Appearance of EL emission in negative cycles of the ac voltage is explained in terms of available residual charges injected in the previous positive cycle of the sinusoidal voltage; the relative intensity of EL emission in the negative cycle can be correlated to the ambipolarity of charge carriers in the CH3NH3PbBrxI3-x series. At low frequencies of the ac voltage, the dynamic response of EL emission in any cycle is in phase with the applied ac voltage; interestingly, the EL emission starts to lag the sinusoidal voltage at higher frequencies, this has been correlated to the ambipolarity of the active perovskite material. Finally, the frequency dependence of EL emission under an ac voltage provides the limiting frequency of device operation (−3 dB frequency) and thereby the effective carrier mobility in the active heterostructure.

PEX4

Towards enhanced room-temperature photovoltaic effect in ferroelectric Bi and Fe codoped $BaTiO_3$

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Abstract

A material with low band-gap (ideally close to ~1.4 eV) and high ferroelectric (FE) polarization can be very promising for photovoltaic applications due to its efficient FE polarization driven charge carrier separation. Additionally, reasonable electrical conductivity also seems desirable from such a material to increase the short circuit current value. However, the above combination is usually contraindicated, and FE materials usually possess very high band-gap (~3-4 eV) and extremely poor electrical conductivity, which renders them unsuitable for photovoltaic applications. Here, we demonstrate that a carefully designed Bi-Fe codoped $BaTiO_3$ (BTO) system ($Ba_{1-x}Bi_xTi_{0.9}Fe_{0.1}O_{3-\delta}$, $0\leq x \leq 0.10$) provides a unique platform where we can have simultaneous optimization of low optical band-gap, high FE polarization and reasonable electrical conductivity. We, thereby, find that the local Jahn-Teller distortion associated with doped transition metal ions, tetragonality (c/a) of the unit cell and oxygen vacancy content lead to a controlled tuning of optical band-gap, FE polarization and electrical conductivity respectively over a wide range. While x=0.00 (only Fe-doped BTO) stabilizes in the undesirable paraelectric-hexagonal phase, x=0.02 (Bi-Fe codoped) composition is engineered to possess an optimized combination of a low band-gap of ~1.55 eV, the largest FE remnant polarization of ~5.2 $\mu C/cm^2$ due to significant recovery of the FE BTO-tetragonal phase by more than ~60 % and reasonably high electrical conductivity compared to $BaTiO_3$, which cause it to exhibit the largest photovoltaic response within the series. Such an approach of optimizing the desired physical properties in a closely related mixed phase material (i.e. a suitable combination of polymorphs) where the optimization of ferroelectricity is engineered in majority tetragonal BTO phase, while the minority hexagonal BTO phase aids in the reasonable electrical conductivity (a combination that is not realizable in a single phase FE material), along with an optimum band-gap, is promising in the realization of many potential ferroelectric based photovoltaic materials.

Comparative Fermiology Study of $PbBi_2Te_4$ and $SnBi_2Te_4$ 3D Topological Insulators

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Abstract

Topological insulators (TIs) are the novel class of materials with insulating bulk and having time reversal symmetry protected conducting boundaries. The unique spin momentum locking of the surface carriers in TIs results in rotation of spins along back scattering paths by an amount π which can qualitatively and quantitatively be confirmed from observation of weak antilcalization (WAL) effect and ½-shift of Landau index in Landau levels fan diagram made from Shubinikov-de Haas (SdH) oscillations, respectively. SdH oscillations with π Berry phase are the signature of presence of Dirac Fermions related to the non-trivial topological surface states in 3D TIs. $PbBi_2Te_4$ and $SnBi_2Te_4$ are predicted to be 3D TIs from density functional theory calculation [1, 2] follows by experimental verification through angle-resolved photoemission spectroscopy (ARPES) measurements for $PbBi_2Te_4$ [3] while to the best of our knowledge Dirac dispersion nature of the surface band structure is yet to set in ARPES measurements for $SnBi_2Te_4$. Very few electronic transport measurements have been done on $(Pb/Sn)Bi_2Te_4$, includes n-type to p-type transition with Sb doping in $PbBi_2Te_4$ [4] and the effect of the cation antisites in $SnBi_2Te_4$ single crystal nano plates [5] etc. The unique π-Berry phase related to Dirac Fermions in TIs are not verified yet for these specimens, motivated us to do transport study of $(Pb/Sn)Bi_2Te_4$ single crystals. Herein, a comparative electronic transport and Hall study of $PbBi_2Te_4$ and $SnBi_2Te_4$ single crystals has done here. Hall measurements reveal Sn acts as an acceptor impurity when replaced from Pb in MBi_2Te_4 (M = Pb/ Sn). Modified Hikami-Larkin-Nagaoka equation describing the observed WAL effect in magnetotransport measurements at different temperatures yields phase coherence lengths (l_f). The fitting parameters describing l_f(T) depicts the presence of two dimensional conducting channels in studied single crystals. Non-trivial topological surface states of both the single crystals are confirmed from the observed ½-shift of Landau index in Landau levels fan diagram, a clear manifestation of the π Berry phase of the carriers. Estimated lower effective masses from the Lifshitz-Kosevich (LK) fit and higher mobility values obtained from Dingle analysis confirms the surface origin of the oscillations of both the single crystals. Comparison of the effective mass, mobility and quantum scattering time obtained from the SdH oscillations depict $PbBi_2Te_4$ to be a superior quality topological insulator over $SnBi_2Te_4$. Elongated surface states are observed in both the crystals which accommodate the topological surface states at the surface of the crystals.

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