SRM
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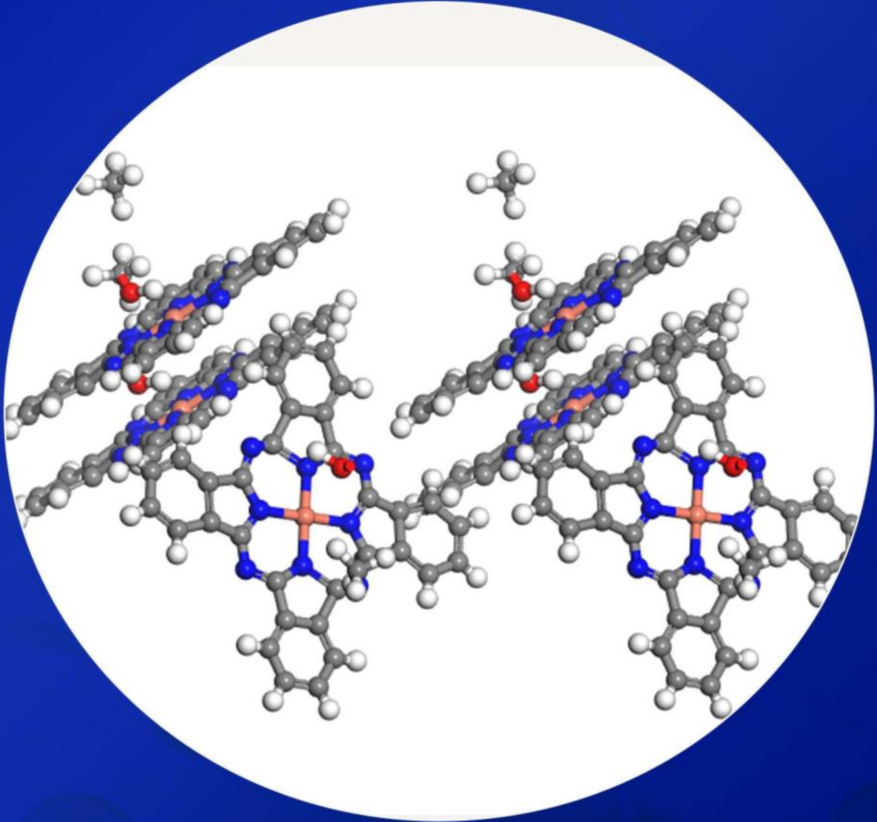
Andhra Pradesh

INTERNATIONAL CONFERENCE ON MATERIALS GENOME (ACCMS-ICMG-II)

SRM University - AP, Andhra Pradesh
March 24-25, 2022



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Objective of the meeting

The enormous leap in computational approaches combined with advances in experimental techniques over the past three decades, demonstrates vividly that this synergy can play a key role in solving challenging problems in Materials Science and Engineering. Quantum Mechanical based calculations complemented by Machine Learning (QM/ML) are ideal to guide experiments in focussed discovery of novel materials with technological potential. The objective of the international conference is to provide a forum for recent advances in experiment, theory, and data science to discover new materials and to understand their fundamental properties. The current status of the field and its future plans and prospects will be highlighted, covering all the recent developments in First-Principles calculations, experiments, materials database and Machine Learning. The objective of this meeting is to promote collaboration not only among theorists but also with experimentalists through the creation, sharing and mining of Data.

RThapa

On behalf of Organizing Committee

Prof. Ranjit Thapa

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Preface

This is the second meeting of the series of International Conference of Materials Genome, ICMG-II. Two years back the first meeting was arranged by Professor Ranjit Thapa at the SRM University-AP, when just COVID-19 problem started. I myself could arrive there, but in between I experienced many strange things, for example I was the only one traveler in the airport connection train! When we started the conference, many of the foreigners could not pass the border, even several people had arrived the Indian airport but were rejected entry. Therefore, several foreign speakers changed to deliver their talks online. At that time we all believed that the bad situation will soon be recovered, but unfortunately it became worse and worse. However, we could overcome this abnormal situation for the international conference without physical travels by using teleconference systems. This time also we utilize it fully and since we are now very much used to this situation, smooth operation of the conference is expected as usual by the support of the University.

It is very successful to have 4 keynote speakers, 53 Invited speakers, 140 total participants, 20 Oral and 23 posters. Maximum 5 parallel sessions will be held. Although no physical contact, please enjoy our warm conference environment in two days.

Just before the 21st century started I invited my 17 good friends to Sendai, Japan from over the world to organize ACCMS. In the inauguration meeting in Sendai. I stated to all my friends that "I have a dream" is a famous statement by Martin Luther King, Jr. to express his idea of unification of black and white people in America. Unfortunately, in 21st century still there is a big economical difference among researchers in all the research fields depending on countries. We are selfish to try to fight with other researchers to obtain better environment aiming to establish only our own good status. Now is the time! We should overcome such selfish consideration and gather together to share resources equally to make research environment more uniform over the world and make people happier.

I am very thankful to all the participants to this meeting from India and oversea and the support by SRM University-AP. Professor Ranjit Thapa and his group have worked out to make this conference an excellent one. I very much appreciate their contribution to this important meeting online.

Yoshiyuki Kawazoe

Yoshiyuki Kawazoe
Founder of ACCMS
Senior Research Fellow
New Industry Creation Hatchery Center, Tohoku University

Special Address

Reliable Ab initio Simulation for Materials Design Fundamentally Better than Present Day Standard for Materials Genome

Prof. Yoshiyuki Kawazoe

New Industry Creation Hatchery Center, Tohoku University, Sendai, Japan

In computational materials science society, a large number of papers are published using ab initio computer simulation software based on DFT (Density Functional Theory) to design new useful materials. However, there is a fundamental problem to apply DFT, since DFT is a complete ground state theory but no power to determine the exchange-correlation functional. In most of the published papers authors apply DFT to analyze experimental observations, which are related to excited states, such as band-gap value. A frequently used terminology of “band gap engineering” based on DFT is theoretically incorrect, since DFT cannot estimate the energy of exited levels such as conduction band (for example, LDA+U is a phenomenology with U fitting parameter). It is known that TD DFT (Time Dependent DFT) or GW approximation help this situation. Although most of the researchers believe that GW approximation is expensive, GW term is a single integral and can be parallelized. Therefore, using the present-day supercomputers having a number of cores (nodes), the wall clock time is not much different from DFT.

Most of *ab initio* simulation packages use pseudo-potential, and therefore absolute energy estimation is not possible, for example, band gap value is possible to be estimated, but not the ionization energy or electron affinity. We have developed TOMBO code (TOhoku Mixe-Basis Orbitals ab initio simulation program package) which is an all-electron full-potential code based on mixed-basis (atomic orbitals and plane waves). By TOMBO we have already solved above mentioned problems, and also made it possible to estimate core related physical/chemical properties such as hyperfine structure constant and NMR chemical shift. Recent progress in TOMBO development is amazing to implement GW+Γ to achieve 0.1eV accuracy in total energy without any parameters, and can trace chemical reaction without adiabatic approximation. (Please join the Professor Kaoru Ohno’s keynote speech in this conference).

One more severe problem is that our subject is “many electrons problem”, and not easy to explain the ab initio numerical results. We have proved two level models, such as frequently used Hubbard model are completely incorrect, since the energy difference between 2 levels (such as magnetic/non-magnetic) arises mainly from the space-wave function difference, not from exchange energy. We should rewrite the traditional textbooks in solid state physics and achieve a predictable theory (from the level of explanation of experimental values, but independent from them; Theory first!).

Recently MI (Materials Informatics) is very popular to be applied to new useful materials design, which is the title of this International Conference as “Materials Genome”. However, the fundamental procedure above mentioned is really necessary to be independent from experimental studies. (Theory first should be realized!) Only based on this level of the theory, MI is really useful and possible to request experimentalists to find out the new materials we predicted with confidence.

Predictive Models for Innovative Design of Materials using Quantum Mechanics and Machine Learning

Prof. Umesh Waghmare
Theoretical Sciences Unit, J Nehru Centre for Advanced Scientific Research, Jakkur PO, Bangalore 560 064 INDIA

We introduce fundamental ideas used in computer simulations based on quantum mechanical description of electronic motion in a material to predict its structure and properties, and illustrate them through demonstration of scale-free ferroelectricity in HfO_2 opening up opportunities of ultimately dense dipolar switching devices directly integrable into silicon technology. To augment the range of applications of such *first-principles* quantum simulations, we present a machine learning scheme that identifies finger-print descriptors of material properties from analysis of relatively *small* data, and develop models of complex material behaviour like dielectric breakdown that often determines failure of electronic devices. These schemes of multi-scale modelling can be combined into an integrated computational approach to design of materials with prediction of evolution of its structure and properties starting from synthesis.

Keynotes

K-01 Pressure Induced Structural Phase Transitions in Layered $EuSn_2As_2$ Compounds

Jian-Tao Wang[1,2,3,], Xiaohui Yu[1,2,3], Fang Hong[1,2,3], Changfeng Chen[4]*

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Abstract:

Pressure, as a basic thermodynamic parameter, plays an important role in the researches of topological materials, and can effectively tune the crystal and electronic structure of material to form a new state of matter. The magnetic topological insulator $EuSn_2As_2$ is known to crystallize in a Bi_2Te_3-type layered structure in rhombohedral symmetry (α-phase, No. 166) at ambient conditions. Combination of *ab initio* calculations and *in-situ* x-ray diffraction measurements, we identify a new monoclinic (C2/m, No. 12) high-pressure structure β-$EuSn_2As_2$ [1] and a new pressure-densified rhombohedral (R-3m, No. 166) structure γ-$EuSn_2As_2$ [2]. The β-$EuSn_2As_2$ has a three-dimensional network made up of honeycomb-like Sn sheets and zigzag As chains, transformed from the layered α-phase via a two-stage reconstruction mechanism with the connecting of Sn-Sn and As-As atoms successively between the buckled SnAs layers, with a strong *shear deformation* assisted expansion along the [210] orientation; while γ-$EuSn_2As_2$ is comprising Sn-As-As-Sn linear chains along the *z*-axis and can be realized via the formation of As-As bonds in the compressed AsSn/SnAs bilayers with a strong anisotropic lattice distortion along the [001] orientation. Also, in layered magnetic $NiPS_3$, a two-stage phase transition from a monoclinic (C2/m) to a trigonal (P-31m, No. 162) lattice is identified in corresponding to a layer-by-layer slip mechanism along the *a*-axis [3]. Moreover, we have studied the electronic and structural phase transitions in the magnetic topological insulator $MnSb_2Te_4$ under hydrostatic pressure [4]. These works have demonstrated the correlation among interlayer interaction, magnetic ordering, and electric behavior.

Keywords: high-pressure; structural phase transition; magnetic phase transition

References:

[1] Lin Zhao, *et al.*, Monoclinic $EuSn_2As_2$: A Novel High-Pressure Network Structure, Phys. Rev. Lett. **126**, 155701 (2021), https://doi.org/10.1103/PhysRevLett.126.155701
[2] Jian-Tao Wang, *et al.*, Pressure-densified new rhombohedral phase of $EuSn_2As_2$, Phys. Rev. B **104**, L220101 (2021), https://doi.org/10.1103/PhysRevB.104.L220101
[3] Xiaoli Ma, *et al.*, Dimensional crossover tuned by pressure in layered magnetic $NiPS_3$, Sci. China-Phys. Mech. Astron. **64**, 297011 (2021), https://doi.org/10.1007/s11433-021-1727-6
[4] Yunyu Yin, *et al.*, Pressure-driven electronic and structural phase transition in intrinsic magnetic topological insulator $MnSb_2Te_4$, Phys. Rev. B **104**, 174114 (2021),

https://doi.org/10.1103/PhysRevB.104.174114

K-02 Atomic semiconductor of ultimate-density via flat phonon bands

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Abstract:

Dispersion-less flat energy bands in momentum space are known to generate localized independent states in real space. We discovered that flat phonon bands exist in ferroelectric HfO_2 and produce an independent motion of atoms as if their chemical bond disappears by an external voltage. With the vanishing bond, each atom can be freely displaced by the voltage for information storage. Our discovery of the direct atom control in a solid will lead us to the design of ultimate-density memory semiconductors reaching up to ~100 TB [1]. Our theory is directly applicable to the Si-compatible HfO_2 so can be materialized in all electronic devices [2]. Just as Einstein's theory of relativity ($E=mc^2$) enabled us to make bombs out of atoms not out of materials, with our "Atomic Semiconductor" we will open the era of operating memories on an atomic scale rather than a materials scale and carrying a data center in the palm of your hand.

Keywords: high-pressure; structural phase transition; magnetic phase transition

References:

[1] "Scale-free ferroelectricity driven by flat phonon bands in HfO_2", H.-J. Lee et al., Science **369**, 1343 (2020).

[2] "A key piece of the ferroelectric hafnia", B. Noheda et al., Science **369**, 1300 (2020).

BIO:

Dr. Jun Hee Lee is a computational physicist/chemist. He obtained his ph.D in physics from Seoul National University in 2008. Then he moved to USA as a postdoc at Physics Dept. of Rutgers U (2008~2011), Chemistry Dept. of Princeton U (2011~2013), and Materials division of Oak Ridge National Lab. (2013~2015). Now he joined UNIST in 2015 as an assistant professor and is an associate professor. Combining his interdisciplinary background, he has been actively working on various fields such as ferroelectrics, multiferroics, polymers, and energy materials including photocatalysts, fuel cells, and batteries. He published 70 SCI papers including a recent theory paper in Science "*Scale-free ferroelectricity by flat phonon bands in* HfO_2", Science **369**, 1343 (2022). Nowadays he is extending his theoretical research across industries to realize ultimate-density semiconductors reaching up to ~100 TB.

K-03 What is so interesting about $A_{1-y}B_yPbX_3$ (A/B = MA, FA, Cs and X = I, Br, Cl)

D. D. Sharma

Solid State & Structural Chemistry Unit, Indian Institute of science, Bengaluru 560012, India.

The last decade has seen the most spectacular rise of the halide perovskites with the general formula of ABX_3, where most commonly A = $(CH_3NH_3)^+$ (MA), $(CH(NH_2)_2)^+$ (FA) or Cs^+, B = Pb^{2+} or Sn^{2+}, and X = I^-, Br^- or Cl^- for their superlative photovoltaic and light emissive properties. $MAPbI_3$ is the most investigated among the pure systems. However, a rapid degradation of its performance has been a vexing issue, ameliorated by *A*-site cationic substitutions, such as in $MA_{1-y}FA_yPbX_3$. However, the microscopic changes brought about by such substitutions are not well understood at present. In this talk, I shall present our efforts at understanding the relevant physical properties of these materials by first investigating the pure end-members, $APbX_3$ (A = MA, FA, or Cs and X = I, Br, or Cl) and then by contrasting these with the A-site cation substituted systems, $A_{1-y}B_yPbX_3$ to unravel several interesting changes.

This work is a result of collaborations with B Bhattacharyya, M Bokdam, C De, J. P. Embs, C Franchini, S Ghara, TN Guru Row, A Hossain, BP Kore, G Kresse, A Kumar, J Lahnsteiner, P Mahale, A Mohanty, S Mukherjee, R. Mukhopadhyay, S Pal, A Pandey, MS Pavan, S Picozzi, T Sander, Sharada G, V. K. Sharma, A Stroppa, A Sundaresan, D Swain and M. Tyagi.

Relevant references:

1. M Bokdam et al., Sci. Rep. **6**, 28618 (2016).
2. J Lahnsteiner et al., Phys. Rev. B **94**, 214114 (2016).
3. Sharada G *et al*., J. Phys. Chem. Lett. **7**, 2412 (2016).
4. Sharada G *et al*., J. Phys. Chem. Lett. **8**, 4113 (2017).
5. Sharada G *et al*., J. Phys. Chem. C **122**, 13758 (2018).
6. A Mohanty *et al.*, ACS Energy Lett. 4, 2045 (2019).
7. V. K. Sharma *et al*., J. Phys. Chem. Lett. **11**, 9669 (2020).
8. V. K. Sharma et al., J. Phys. Chem. C 125, 13666 (2021).

K-04 Extended Kohn-Sham theory applicable to arbitrary excited eigenstates

Kaoru Ohno[1]

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Abstract:

To simulate solar cells, photo-induced chemical reactions, OER/HER/ORR, X-ray processes, etc., one has to calculate excited states, for which density functional theory (DFT) is not applicable. Although time-dependent density functional theory (TDDFT) is applicable, the exchange-correlation kernel is unknown as a function of the initial excited state of the system. A possible strategy is to use extended quasiparticle (EQP) theory, which can treat the photoemission (PE) or inverse photoemission (IPE) process for an initially excited eigenstate [1]. However, there has been a long-standing problem that the quasiparticle wave functions have a norm smaller than 1. That is, even for a finite *N* electron system, one has to treat infinite number of occupied quasiparticle wave functions. This makes the treatment very difficult. Quite recently, we have succeeded in solving this problem by introducing extended Kohn-Sham (EKS) theory [2]. According to EKS theory, one can simply omit quasiparticle wave functions involving multiple excitations, and simply normalize quasiparticle wave functions associated with the pure hole or electron state created by the PE/IPE process. The simplest way to adopt EKS theory is to apply the one-shot GW approximation to an initially excited state. In my talk, I will demonstrate several successful examples of the excited state calculations.

[1] K. Ohno, S. Ono, and T. Isobe, J. Chem. Phys. 146, 084108 (2017).
[2] T. Nakashima, H. Raebiger, and K. Ohno, Phys. Rev. B 104, L201116 (2021).

Keywords: first-principles, quasiparticle theory, Kohn-Sham theory, excited states

Invited Speaker

IL-01: Machine learning assisted development of 2DMatPedia

Dr. Jun Zhou,
IMRE, Singapore

In the past few years, we have established an in-house database with quantum simulation results of 2D materials, called 2D Materials Encyclopedia (2DMatPedia). In this open database, we have accumulated the data of the basic properties for more than 6000 2D materials. Leveraging these highly consistent data, we trained machine learning (ML) models to further develop our database. a) A model is trained to predict the decomposition energies of *unrelaxed* 2D materials. This allows us to prescreen the potentially stable candidates from the >180,000 new ternary compounds generated for further high-throughput first-principles simulations. Around 1/3 of these compounds are found to be stable. b) We first screen 83 2D magnetic materials from 2DMatPedia and identify their magnetic ground states. ML models is developed to classify the 2D materials into the respective categories of non-magnetic and magnetic materials with an accuracy of 93.4%, the latter of which is further classified into antiferromagnetic and ferromagnetic materials with an accuracy of 94.4%. A web AI application for predicting magnetism of 2D materials has been developed and can be found at https://twodferromagnetism-model.herokuapp.com.

IL-02: ML Assisted Knowledge Discovery

Prof. Abhishek Kumar Singh,

Indian Institute of Science, Bangalore, India

Data driven machine learning methods in materials science are emerging as one of the promising tools for expanding the discovery domain of materials to unravel useful knowledge. In this talk, the power of these methods will be illustrated by covering three major aspects, namely, development of prediction models, establishment of hidden connections and scope of new algorithmic developments. For the first aspect, we have developed accurate prediction models for various computationally expensive physical properties such as band gap, band edges and lattice thermal conductivity. The prediction model for band gap and band edges are developed on 2D family of materials -MXene, which are very promising for a wide range of electronic to energy applications, which rely on accurate estimation of band gap and band edges. These models are developed with GW level accuracy, and hence can accelerate the screening of desired materials by estimating the band gaps and band edges in a matter of minutes. For the lattice thermal conductivity prediction model, an exhaustive database of bulk materials is prepared. By employing the high-throughput approach, several ultra-low and ultra-high lattice thermal conductivity compounds are predicted. The property map is generated from the high-throughput approach and four simple features directly related to the physics of lattice thermal conductivity are proposed. The performance of the model is far superior than the physics-based Slack model, highlighting the simplicity and power of the proposed machine learning models. For the second aspect, we have connected the otherwise independent electronic and thermal transport properties. The role of bonding attributes in establishing this relationship is unraveled by machine learning. An accurate machine learning model for thermal transport properties is proposed, where electronic transport and bonding characteristics are employed as descriptors. In the third aspect, we have proposed a new algorithm to develop highly transferable prediction models. The approach is named as guided patchwork kriging, which is applied for prediction of lattice thermal conductivity.

References:

1. Chemistry of Materials 30, 4031, 2019
2. Journal of Physical Chemistry Letters 10, 780, 2019
3. Chemistry of Materials, 31, 5145, 2019
4. Journal of Materials Chemistry A 8, 8716, 2020
5. Journal of Physics: Materials 3, 024006, 2020

IL-03: Machine Learning Approach of Design of New Materials with Targeted Properties

Dr. Tanusri Saha -Dasgupta
S. N. Bose National Centre for Basic Sciences, Kolkata, India

One of the strong pillars in advancement of designed materials, with targeted properties like magnetism, superconductivity, topological characters is computation of materials. The synthesis and optimization of properties of real materials in experiment is both time-consuming and costly, being mostly based on trial and error. Computational approach in this connection is of natural interest to screen materials, before they can be suggested and tested in the laboratory. For the prediction of new materials, a powerful tool is the machine-learning assisted high throughput computation. In this approach new materials have been computationally predicted by combining electronic-structure methods with intelligent machine learning technique based on data mining and database construction. In this talk we discuss application of this method for prediction of new magnetic double perovskites [1], low cost rare earth based permanent magnets [2] and semiconductor heterostructures.[3]

References:

[1] Halder A, Ghosh A, and Saha Dasgupta T 2019 *Phys. Rev. Materials* 3, 084418.
[2] Halder A, Rom S, Ghosh A, and Saha-Dasgupta T 2020 *Phys. Rev. Applied* 14, 034024.
[3] Rom S, Ghosh A, Halder A and Saha-Dasgupta T 2021 *Phys. Rev. Materials 5*, 043801.

IL-04: Machine learning-assisted Ab-initio Random Structure Searching (AIRSS): Preliminary application to Sodium-VS_2 system for NIBs

Prof. Darwin Putungan,
University of Phillipines, Phillipines.

In this talk, I will present how the simple but elegant method Ab-initio Random Structure Searching (AIRSS) is used to make more accurate predictions of important energy storage metrics such as specific energy capacity and open circuit voltage for metal-ion batteries. I will also discuss the important limitations of the method, and how machine learning can significantly help in making the method more powerful and computationally less expensive for larger systems.

Biosketch:

Darwin Putungan obtained his PhD in Physics degree from the National Taiwan University in collaboration with the Institute of Physics and the Institute of Atomic and Molecular Sciences of Academia Sinica under the Taiwan International Graduate Program (TIGP) fellowship. He is currently a professor at the Physics Division, Institute of Mathematical Sciences and Physics (IMSP) and a Junior Associate of the Condensed Matter and Statistical Physics Group at The Abdus Salam International Center for Theoretical Physics in Trieste, Italy. He is a member of the Materials Computation Research Group under the Condensed Matter and Statistical Physics Cluster of the Physics Division. His research interests include computational research studies on 2D materials for energy conversion and storage, kinetic Monte Carlo simulations and just recently, he became interested in utilizing machine learning in the study of materials structures for important applications.

IL-05: Applied Machine Learning and DFT for alloys, additive manufacturing and beyond …

Dr. Maaouia Souissi,
Brunel University London, United Kingdom.

Artificial intelligence and machine learning (AIML) could add £630 billions to the UK economy by 2035, increasing the annual growth rate of the gross value added from 2.5 to 3.9% [1]. The aluminum and steel industries will have a significant contribution to this growth. For high-strength aluminum alloys, for instance, an Al-Zn-Mg-Cu alloy (7xxx series) with a high ultimate tensile strength of 952 MPa was developed by ML composition optimization and process optimization [2]. Generally, the development and analysis of a new alloy are conducted on a trial-and-error basis, which requires a systematic production of alloys with varied compositions and heat treatments until one finds the most suitable alloy for an application. This approach is often costly and time-consuming, especially for multicomponent alloys. Recently, experiments are also heavily affected by social distancing. With the improved understanding of the structure-composition property relationship and incorporating the thermodynamic conditions, together with more powerful and reliable modern computational techniques, alloy design is increasingly oriented to the computational prediction and experimental validation. In this regard, to develop and establish advanced procedures compared to the existing standard methods, using ML, we will show case studies of property-oriented alloy prediction schemes from collected experimental data. Once the optimum material has been found by the ML model, density functional theory (DFT) will be employed for a deeper fundamental understanding of the physical interactions and chemical bonding at the atomic level mainly contributing to the overall good performance of the material discovered before the final recommendation for experimental characterization.

Keywords: Al-based alloys; steels; alloy design, AIML and DFT.

References

[1]https://assets.publishing.service.gov.uk/government/uploads/system/uploads/attachment_data/file/652097/Growing_the_artificial_intelligence_industry_in_the_UK.pdf#:~:text=Growing%20the%20Artificial%20Intelligence%20Industry%20in%20the%20UK,higher%20accurac

[2] J. Li et al. Commun. Mater. 1 (2020) 73.
https://www.nature.com/articles/s43246-020-00074-2

IL-06: Combining Machine Learning with high throughput first principles calculations to analyse the charge and heat transport in thermoelectric solid

Dr. Amrita Bhattacharya,
Indian Institute of Technology, Bombay, India.

Thermoelectrics are viable alternative towards achieving a green energy economy. First principles density functional theory calculations may aid to the issue of cost effective deployment of efficient thermoelectric materials by enabling a rapid prescreening of the preriodic table prior to their synthesis in the laboratory. On the other hand such calculations may reveal underlying complex interplay of electronic and vibrational transport phenomena. Focussing on half Heusler materials class (XYZ), we perform high throughput calculations to investigate the effect of isovalent subsitution of elements at the X, Y and Z sites in the transport properties of stable half Heusler compounds [1]. Thereby, we show that Y site doping is detrimental for enhancing the electronic transport coefficients. However, we find that a small amount of off stoichiometric excess self doping with the Y site elements in these half Heusler compounds, may lead to drastic lowering of the lattice thermal conductivity [2,3]. Further, we use machine learning to predict the lattice thermal conductivity of semiconducting half Heusler compounds [4].

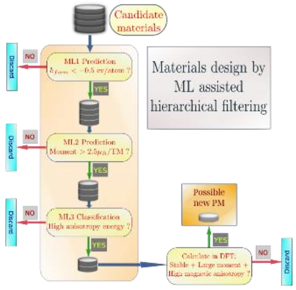
References:

1. P. R. Raghuvanshi, Suman Mondal, and Amrita Bhattacharya, “A high throughput search for efficient thermoelectric half-Heusler compounds”, Journal of Materials Chemistry A, 8 , 25187 (2020)
2. Nagendra S. Chauhan, Bhasker Gahtori, Bathula Sivaiah, Subhendra D. Mahanti, Ajay Dhar, and Amrita Bhattacharya*, "Modulating the lattice dynamics of n-type Heusler compounds via tuning Ni concentration", Appl. Phys. Lett., 113, 013902 (2018).
3. P. R. Raghuvanshi, D. Bhattacharya, and Amrita Bhattacharya, “Self-Doping for Synergistically Tuning the Electronic and Thermal Transport Coefficients in n-Type Half-Heuslers”, ACS Applied Materials & Interfaces, 13, 55060 (2021).
4. D. Bhattacharya, K. Kundayu, D. Saraswat, P. R. Raghuvanshi and Amrita Bhattacharya, “A thorough descriptor search to machine learn the lattice thermal conductivity of half-Heusler alloys”, ACS applied energy materials (2022).

IL-07: Machine Learning assisted hierarchical screening: A strategy for designing novel magnetic materials

Dr. Prasenjit Sen,
Harish-Chandra Research Institute, Prayagraj (Allahabad), India.

Designing permanent magnets (PM) without rare earth (RE) elements is both a strategic imperative and a fundamental challenge. Material design has traditionally relied on the trial-and-error approach. This is, however, tedious, time consuming, expensive and also uncertain. Recently a number of materials databases have started come up, with a wide range of properties, particularly after the launch of the Materials Genome Initiative. This has made application of Machine Learning methods to the question of materials design and discovery an attractive proposition.



In this talk I will present our work on application of Machine Learning to the problem of developing PMs without RE elements. We have developed Machine Learning models to hierarchically filter and select stable magnetic materials with large magnetization and magnetic anisotropy energy. These models are trained on the c2db dataset of two dimensional (2D) materials obtained from the Computational Materials Repository (CMR). Starting from an initial set of 278 novel 2D materials, the models identify 10 to satisfy the desired target properties of stability, large magnetic moment and large anisotropy energy. Subsequent first principles calculations based on density functional theory establish that the model predictions are quite accurate. This establishes the first step towards a complete ML-assisted design of RE free PMs.

References:

[1] Designing rare earth free permanent magnets: insights from small Co clusters, A. Sen and P. Sen, PCCP 21, 22577 (2019).

[2] Machine learning assisted hierarchical filtering: a strategy for designing magnets with large moment and anisotropy energy, A. Dutta and P. Sen, J Mater. Chem. DOI: 10.1039/d1tc03776e

IL-08: In-silico Design of Novel Catalytic Materials using ab-initio Microkinetic Modeling Augmented with Machine Learning

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Rational design of heterogeneous catalysis is immensely important to modern and future society. It forms the foundation of the chemical industry, supplying essential chemicals and commodities for transport, food production, and pharmaceuticals, and is also a cornerstone in current and future energy platforms. Understanding surface science has always been essential for the rational design and development of catalytic materials for industrial chemical processes. Computational approaches, particularly density functional theory (DFT) play an increasingly important role in modern surface science and catalysis. In-silico design of catalytic materials for industrially relevant processes by combining ab-initio DFT calculated reaction energies and activation barriers in combination with microkinetic modeling have been shown to be highly promising [1, 2, 3]. The use of a descriptor based approach, where the activity and selectivity of a catalyst are represented by binding energies of adsorbate species has been widely used to screen new materials with better activity, selectivity, and stability.

In our recent studies, we have been working on augmenting the machine learning tools with the ab-initio microkinetic modeling to speed up the in-silico catalyst screening process and also understand how the common periodic table features modulate the catalyst activity[4]. The Gradient Boosting Regression (GBR) algorithm was found to be the most successful ML method for catalyst screening, especially while working with a small dataset. The applicability of the ML method was demonstrated in two distinct cases. In the first case, GBR based ML model was used to calculate the carbon and oxygen binding energies over the A_3B bimetallic alloys, which were then combined with ab-initio microkinetic modeling to calculate the catalytic activity trends for hydrodeoxygenation of ethanol to ethane[4] and dehydrogenation of ethanol to acetaldehyde [4]. The dehydrogenation of ethanol to acetaldehyde reaction was further expanded to single atom alloy (SAA) surfaces of Au, Ag, and Cu based bimetallic alloys using the combined ML and ab-initio MKM methods[5, 6]. In the second case study, the same GBR algorithm is applied to estimate the deprotonation energies of heteropolyacid ($H_nM_{12}XO_{40}$) catalysts, when the addenda M atom is varied between W and Mo and the central atom X from the p-block elements. Deprotonation energies of HPAs are often applied as reactivity descriptors for acid-catalyzed reactions like esterification, dehydration, etc. [7]. In both cases, easily available element properties were used as input features while ensuring good accuracy in the prediction of the reactivity descriptors.

References:

1. Yue Xu, Adam C. Lausche, Shengguang Wang, Tuhin S. Khan, Frank Abild-Pedersen, Felix Studt, Jens K. Nørskov, Thomas Bligaard, “In silico Search for Novel Methane Steam Reforming Catalysts” New Journal of Physics, 15, 125021, 2013

2. Fatima Jalid, Tuhin Suvra Khan, Fasil Qayoom Mir, and M. Ali Haider, “Understanding Trends in Hydrodeoxygenation Reactivity of Metal and Bimetallic Alloy Catalysts from Ethanol Reaction on Stepped Surface”, Journal of Catalysis, 353, 265-273, 2017
3. Tuhin S. Khan, Fatima Jalid, M. Ali Haider, “First-Principle Microkinetic Modeling of Ethanol Dehydrogenation on Metal Catalyst Surfaces in Non-oxidative Environment: Design of Bimetallic Alloys”, Topics in Catalysis, 61, 1820–1831, 2018
4. Shivam Saxena, Tuhin S. Khan, Fatima Jalid, Manoj C. Ramteke, M. Ali Haider, “In Silico High Throughput Screening of Bimetallic and Single Atom Alloys Using Machine Learning and Ab Initio Microkinetic Modelling”, Journal of Materials Chemistry A, 8, 107-123, 2020
5. Amrish Kumar, Jayendran Iyer, Fatima Jalid, Manojkumar Ramteke, Tuhin S. Khan, M. Ali Haider, “Machine Learning Enabled Screening of Single Atom Alloys: Predicting Reactivity Trend for Ethanol Dehydrogenation”, ChemCatChem, 14, e202101481, 2021
6. Jayendran Iyer, Fatima Jalid, Tuhin S. Khan, M Ali Haider, “Tracing the reactivity of single atom alloys for ethanol dehydrogenation using ab initio simulations”, Reaction Chemistry & Engineering, 7, 61-75, 2022
7. Ejaz, Ahmad, Tuhin S. Khan, Md. Imteyaz Alam, K. K. Pant, M. Ali Haider, “Understanding Reaction Kinetics, Deprotonation and Solvation of Brønsted Acidic Protons in Heteropolyacid Catalyzed Synthesis of Biorenewable Alkyl Levulinates”, Chemical Engineering Journal, 400, 125916, 2020

IL-09: Adaptive Learning, Model Interpretability and Bayesian Inference for Accelerating Materials Design

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In our group, we are currently exploring two ways to leverage data science-based approaches in materials design. The first approach takes a data-driven motivation. The domain knowledge is incorporated in the form of physically-motivated descriptors. Machine learning methods are integrated with optimal learning methods to efficiently navigate the vast search space in an adaptive or iterative manner. One of the expected outcomes from adaptive learning is a predictive black-box machine learning or surrogate model that is believed to capture the complexity of the structure-property relationships with sufficient accuracy. More recently, our group has been integrating novel post hoc model interpretability methods to peek inside the trained surrogate models and explain the predictions for each observation in the training data. The second approach combines experimental data with numerical or analytical models within the framework of Bayesian inference. In this talk, I will focus on specific examples that highlight the potential of both approaches in accelerating new materials design.

IL-10: Theoretical Strategies and Methodologies for Investigating Electrocatalytic Reactions (HER/OER/ORR/IRR) on Nanostructures

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Abstract:

Heteroatom-incorporated carbon materials and heterojunction nanostructures have demonstrated significant interest as electrocatalyst due to their tunable surface chemistry and electronic structures. And computational approaches have provided rational interpretation and theoretical insight for the design of novel high-performance catalysts. In the recent developments of various carbon-based 2D materials and heterojunction nanostructures, we proposed and emphasized the synergistic effect between the geometric and electronic effects of these catalysts resulting in the improved catalytic activities. The intentionally induced structural curvature or lattice strain can increase active sites on the surface, even activate inert sites also, and remarkably enhance the catalytic activity by controlling the electronic structure, such as p-/n-type doping, d-/p-band center shift and charge transfer. Based on the theoretical key factors for high-performance catalysts, we propose strategies to develop new catalysts by modifying natural mineral materials. In addition, we explored a new methodology called "one probe and non-equilibrium surface Green's function (OPNS)" to overcome the limitations of free energy diagram (FED) calculation using slab model and to clearly elucidate catalytic reaction mechanisms.

Keywords: Curvature, Heterojunction, Charge transfer, Surface Green function

IL-11: Two-Dimensional Group-IV Carbides for Nanoelectronics and Photocatalytic Water Splitting

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Exploring novel materials with superior properties is of a great significance for potential applications in future nanoelectronics and optoelectronics. Based on first-principles calculations, we predict novel two-dimensional (2D) group-IV carbides containing isolated C2 dimers rather than individual carbon atoms, offering novel properties. We demonstrate that the 2D carbides (XC2, X = Si, Ge, Sn, and so on) have excellent energetic, dynamical, thermal, and mechanical stability with remarkable properties. For penta-carbides, the high specific surface areas, suitable and sizable band gaps, appropriate band edges, small effective carrier masses, and excellent optical absorption capability, all these exotic properties taken together, make them promising candidates for photocatalytic water splitting. On the other hand, their tetrahex counterparts are extremely attractive semiconductors for nanoelectronics. They exhibit narrow direct band gaps, which can be continuously tuned by strain and alloy engineering, and excellent transport properties including strong anisotropic effective mass and ultrahigh (up to 105 cm2 V-1 s-1) carrier mobility. Remarkably, the anisotropy of the carrier effective mass can be rotated by 90° simply by alloying X element or strain engineering in tetrahex carbon. Combining those advanced features, our proposed penta- and tetrahex-carbides are both promising candidates for nanoelectronics and optoelectronics in the future.

Keywords: 2D Materials; Carbides; Nanoelectronics; Optoelectronics; Photocatalytic Water Splitting

IL-12: MXene Based Hybrid Materials for Energy Conversion and Storage Applications

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Rational construction of hybrid nanostructures is one of the efficient approach to design high-performance and flexible energy conversion and storage devices. However, the achievement of improved electrochemical energy conversion and storage storage performance and low-cost production are challenging aspects for scalable production. Recently, MXene a new class of 2D materials has been explored for energy related applications due to their high catalytic and pseudocapacitive properties. These materials are denoted as $M_{n+1}X_nT_x$ (M is transition metals, X is carbon/nitrogen and T is surface terminal groups) which include transition metal carbides, nitrides and carbonitrides derived from bulk MAX phase (clay). To exploit MXene for various applications such as supercapacitors, batteries, catalysis, sensors for biomedical and electromagnetic fields, experimental and theoretical research have been carried out extensively worldwide. Typically, Ti_3C_2 MXene has unveiled better in-plane electrical conductivity (~6500 S cm^{-1}), high electro-active surface area, excellent pseudocapacitive properties, quick charge-transfer kinetics, stability and hydrophilicity with metallic conductivity. In my talk, I'll present the recent research activities and achievements of our research group on design of MXene based hybrid materials for high performance electrocatalyst (HER, OER) and supercapacitor applications.

Keywords: HER, OER, Energy storage, Supercapacitor, 2D materials, MXene

IL-13: Two-dimensional $NbSe_2H$/g-ZnO van der Waals heterostructures as a water splitting photocatalyst: A first-principles study.

Dr. Yeoh Keat Hoe,
Universiti Tunku Abdul Rahman, Malaysia.

Based on first-principles calculations, we propose a new two-dimensional (2D) van der Waal (vdW) heterostructure that can be used as a photocatalyst for water splitting. The heterostructure consists of vertically stacked 2D $NbSe_2H$ and graphene-like ZnO (g-ZnO). Depending on the stacking orders, we identified two configurations that have high binding energies with the energy band gap > 2.6 eV. These 2D systems form a type-II heterostructure which enable the separation of photoexcited electrons and holes. Our study also shows that the 2D NbSe2H/g-ZnO vdW heterostructure has good thermodynamic properties for water splitting. Furthermore, the optical absorption of the 2D NbSe2H/g-ZnO vdW heterostructure extends into the visible light region. Our results suggest that the 2D NbSe2H/g-ZnO vdW heterostructure is a promising photocatalytic material for water splitting.

Keywords: First-principles, 2D $NbSe_2H$, photocatalyst, type-II heterostructure

IL-14: Dynamics of H_2O Dissociation on Metal Surfaces

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Dissociation of H_2O on a metal surface is rate-limiting step in many industrially important reactions. In a few recent experiments, it has been observed that dissociation of H_2O on a metal surface is mode-selective. In other words, this reaction is not statistical in nature and therefore, one cannot use transition state - based theories to get insights of this reaction. Our quantum dynamical calculations show that mode-mode coupling along the reaction path is the key factor in deciding the quantum of mode-selectivity in this reaction.

IL-15: Mechanisms of oxidation of pure and Si-segregated Ti surfaces

Prof. Ryoji Sahara,
National Institute for Materials Science (NIMS), Japan

Titanium and its alloys are used for high-temperature components of jet engines. Their high affinity for oxygen, particularly at elevated temperatures, severely limits their application above 650℃. Using first-principles molecular dynamics, we identified the mechanisms of the oxidation of α-Ti surfaces. Si segregation was found to suppress α-case formation in Ti, which was also confirmed experimentally. Charge transfer from the metal atoms to the gas molecules drives the initial stages of oxidation on the pure and Si segregatedα-Ti (0001) surfaces, while during the later stages, oxidation proceeds via oxygen penetration into the slab. Growth of the oxide network was strongly dependent on the oxidation state of the surface Ti atoms. Oxide growth in the Si-segregated material was retarded with the formation of TiO_x on the surface.

Further, we built a machine learning model to predict the parabolic rate constant, k_p, for high temperature oxidation of Ti alloys. Exploring the experimental studies on high-temperature oxidation of Ti alloys, we built our dataset for machine learning. Apart from the alloy composition, we included the constituent phase of the alloy, temperature of oxidation, time for oxidation, oxygen and moisture content, remaining atmosphere (gas except O_2 gas in dry atmosphere), and mode of oxidation testing as the independent features, while k_p was predicted as the target feature.

The knowledge gained from the study can be used to design novel Ti alloys with excellent resistance towards high-temperature oxidation.

References:
[1] Somesh Kr. Bhattacharya, Ryoji Sahara, Satoshi Suzuki, Kyosuke Ueda, Takayuki Narushima, Appl. Surf. Sci. 463 (2019) 686-692.
[2] Somesh Kr. Bhattacharya, Ryoji Sahara, and Takayuki Narushima, Oxidation of Metals 94 (2020) 205-218.

Keywords: titanium alloys, high temperature materials, oxidation, first-principles calculations, machine learning, parabolic rate constant

IL-16: Electronic Structure of Titania Surfaces Modified by Metal Clusters for Applications in Photocatalysis

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Metal clusters with a size of less than 100 atoms are suitable for modifying the electronic properties of semiconductor surfaces. [1, 2, 3] Such cluster modified surfaces can be used as photocatalysts for various reactions, amongst them for water splitting. In order to avoid agglomeration of the metal clusters and in order to retain their specific electronic structures, the coverage of the surface with metal clusters has to be kept below 10%. The main challenges in this field are a) to maintain the size and thus the properties of the metal clusters and b) to determine the electronic structure of the clusters.

The first challenge described above is considered as one of the main challenges in the field of surface modification with metal clusters can be addressed by introducing defects on the metal oxide surface, specifically oxygen vacancies. The second challenge can be addressed by using experimental techniques which are exclusively sensitive for the electronic structure of the outermost layer. Metastable Induced Electron Spectroscopy (MIES) is such a technique and has been used successfully to determine the change in electronic structure due to the deposition of Au and Ru clusters. Applying techniques such as singular value decomposition, the changes of the electronic structure can even be quantified. [2]

References:

1. D. P. Anderson, J. F. Alvino, A. Gentleman, H.Al Qahtani, L. Thomsen, G. F. Metha, V. B. Golovko, and G. G. Andersson, PCCP **15** (2013) 3917.
2. G. G. Andersson, V. B. Golovko, J. F. Alvino, T. Bennett, O. Shipper, S. M. Mejia, H. Al Qahtani, R. Adnan, N. Gunby, D. P. Anderson, and G. F. Metha. J. Chem. Phys. **141** (2014) 014702.
3. G. Krishnan, H. S. Al Qahtani, J. Li, Y. Yin, N. Eom, V. B. Golovko, G. F. Metha, G. G. Andersson, J. Phys. Chem. C, **121** (2017) 28007.

IL-17: Heterostructures as efficient electrocatalysts for water splitting

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The realization of hydrogen based green economy requires cost effective and highly efficient electrocatalysts, which can lower the energy barriers of both hydrogen and oxygen evolution reactions (HER & OER) involved in water electrolysis. However, high costs of benchmark catalysts based on noble metals are the practical bottleneck for their large scale use. Earth abundant transition metal (TM) based electrocatalysts have quickly emerged as low-cost alternatives, however, the performance and operational stability of these catalysts are still lagging behind the noble metal based counterparts. Out of the all possible approaches implemented to date, development of nano-heterostructures with tuned morphology and suitable electronic coupling is considered as one of the most effective strategy to improve the catalytic efficiency of TM based catalysts. In this talk, HER and OER catalysts based on one and two-dimensional (1D&2D) heterostructures will be discussed. Different solution based strategies to develop size and morphology tuned heterostructure will be presented. Particularly, molecular diffusion controlled interfacial nano-structuring, and selenization induced dealloying of mixed-metal-oxide for heterostructure development will be discussed. In this connection, TM-metal organic framework (TM-MOF)-graphene nanohybrids, TM-selenide based heterostructure, and single atom iridium (SAC-Ir) linked heterostructure will be introduced as efficient HER and OER catalysts. An interesting process of in-situ atomic rearrangement during OER process will be presented and the role of this surface activation process in enhancing the catalytic efficiency will be also discussed. A direct correlation of the experimental results with the theoretical predictions based on density functional theory (DFT) calculations will also be presented.

IL-18: Electrochemical ammonia synthesis through nitrogen reduction reaction on metal phthalocyanine nanostructures

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Electrochemical Ammonia synthesis by nitrogen reduction reaction at ambient conditions can substitute the century old Haber - Bosch process; which results in global 2% carbon dioxide emissions annually. However the electrochemical nitrogen reduction reaction (ENRR) process suffers poor yield rate of ammonia and lower faradic efficiency. Thus the solution lies in the design of specific active site generation of the electrocatalyst for enhanced ENRR performance. Herein, we demonstrate metal phthalocyanine (MPc) nanostructure such as Cobalt phthalocyanine (CoPc) nanotubes, Nickel phthalocyanine (NiPc) nanorods, having well-defined MN_4 configuration as a model electrocatalyst for ENRR due to the greater number of active sites, specificity and selectivity. The chemically synthesized CoPc and NiPc nanostructures showed ammonia yield rate of 108 & 85 $\mu g\ h^{-1}\ mg^{-1}{}_{cat}$ and Faradic efficiency of 28 & 25 % at -0.3 V vs. RHE respectively using 0.1 M HCl as an electrolyte. [1-2]

References:

[1] U. K. Ghorai*, S. Paul, B. Ghorai, A. Adalder, S. Kapse, R. Thapa, A. Nagendra and A. Gain, “Scalable Production of Cobalt Phthalocyanine Nanotubes: Efficient and Robust Hollow Electrocatalyst for Ammonia Synthesis at Room Temperature” ACS Nano 2021, 15, 3, 5230–5239

[2] S. Murmu, S. Paul, S. Kapse, R. Thapa, S. Chattopadhyay, N Abharana, S. N Jha, D. Bhattacharyya, U. K. Ghorai*, “Unveiling the genesis of the high catalytic activity in nickel phthalocyanine for electrochemical ammonia synthesis”, Journal of Materials Chemistry A, 2021, 9, 14477-14484

IL-19: Combined *In Situ* XAS and DFT Studies on the Role of Pt in Zeolite-Supported Metal Catalysts for Selective *n*-Hexane Isomerization

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In this study, we used several in situ, and spectroscopy analyses to investigate the roles of platinum (Pt) in zeolite-supported Pt catalysts for selective n-alkane isomerization. HY zeolites were synthesized using the rice husk silica and impregnated with Pt precursor by incipient wetness impregnation. Typically, HY zeolites have proved to be active hydrocarbon cracking catalysts. The particular challenge is to find an effective catalyst, which favors the isomerization of n-alkanes without too much cracking. In this work, adding Pt atoms to HY zeolite provides an enhanced multifunctional catalyst for converting n-alkanes to branched hydrocarbons. To understand the effect of Pt, we further investigated the reaction mechanism of n-hexane isomerization to 2 methylpentane (2MP) and 3-methylpentane (3MP) by DFT simulations, using a cluster of 30T HY zeolite modeled through B3LYP+3D calculations. We found that, at 450 °C, the isomerization on Pt-HY gives higher cracking products. Decreasing temperature to 300 °C yielded greater selectivity of branched hydrocarbons. In addition, DFT calculations demonstrate that the 2MP production via route A1 (C3–C4 bond activation) and a rate-determining step of 0.97 eV proved more thermodynamically and kinetically favorable than the 3MP product. This agrees well with our experimental observations. Consequently, the presence of Pt on the HY zeolite plays an essential role in both C–C forming and breaking. Finally, the Pt HY zeolite is an efficient catalyst for petroleum production, improving the octane number for catalytic performance and product selectivity by isomerizing straight-chain alkanes to their branched chain isomers.

Keywords: Hexane isomerization, Pt-HY zeolite, in situ CO_2-TPD, DFT, in situ XAS

IL-20: Can we understand CO_2 electroreduction activity of 3d-transition metal atom doping on ZnO monolayers from their oxidation state?

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Single-atom catalyst (SAC) obtained by doping a transition metal (TM) atom to stable monolayers is a promising way to improve CO_2 reduction reaction (CRR) performance. Here we theoretically investigated the CRR activity of 3d-TM doping on ZnO (0001) monolayer (TM-ZnO where TM is Sc, Ti, V, Cr, Mn, Fe, Co, Ni, and Cu). We found that pristine ZnO monolayer requires a high limiting potential of -1.2V to produce HCOOH. On the other hand, we find that doping TMs can significantly reduce the overpotential for CRR. Indeed, Co-ZnO can produce HCOOH with a limiting potential of -0.27 V. Looking at all the 3d-TM, we found that the position in the periodic table of TMs resulted in a difference in reactivity, reaction pathway, and selectivity of the final products. *Early TMs* (Sc to Cr) preferred CH_4 as a product, while late TMs (Mn to Cu) favored producing HCOOH. We tried to understand this difference in reactivity by analyzing the d-orbital occupation of the TM.

Keywords: transition metal atom doping; CO_2 reduction reaction; oxidation state

IL-21: Next-generation smart nanomaterials for electrochemical oxygen and nitrogen reduction reactions

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Over the past several decades, the design and development of advanced electrocatalysts for efficient energy conversion technologies have been subjects of extensive study. With the discovery of two-dimensional nanomaterials, several catalysts have emerged as some of the most promising candidates for heterogeneous electrocatalysis such as such as oxygen and nitrogen reduction reactions due to their unique physical, chemical, and electronic properties. We have extensively worked on different avenues for 2D-nanomaterial development and rendered their advantages towards the electrocatalytic processes both from structural as well as mechanistic point of view. With the unique advances in 2D electrocatalysts based on different compositions and functions followed by specific design principles, oxygen reduction and nitrogen reduction are extensively studied. We have emphasized on different defect and interface engineering strategies for nanomaterials and the influence of these strategies on intrinsic material performance, such as electronic properties and adsorption energetics. We have featured the opportunities of these versatile class of materials as efficient electrocatalysts by considering theoretical calculations, surface characterization, and electrochemical tests. We thereby described the fundamental relationships between electronic structure, adsorption energy, and apparent activity for a wide variety of electrocatalysts with the goal of providing a better understanding of these emerging nanomaterials at the atomic level.

Acknowledgement: R.S.D. acknowledges DST INSPIRE (DST/INSPIRE/04/2015/000337), DST SERB EMR (EMR/2016/000040) and DST SERB (CRG/2020/005683) funding agencies for financial support.

References:
1. M. Das, A. Biswas, R. S. Dey, *Chem. Commun.,* 2022,58, 1934-1937.
2. A. Biswas, S. Nandi, N. Kamboj, J. Pan, A. Bhowmik, R. S. Dey, *ACS Nano* 2021, 15, 12, 20364–20376.
3. A. Biswas, S. Sarkar, M. Das, N. Kamboj, R. S. Dey, *Inorg. Chem.* 2020, 59, 22, 16385–16397.
4. S. Sarkar, A. Biswas, T. Purkait, M. Das, N. Kamboj, R. S. Dey, *Inorg. Chem.* 2020, 59, 7, 5194–5205.
5. S. Sarkar, A. Biswas, N. Kamboj, R. S. Dey, *Inorg. Chem.* 2020, 59, 18, 13453–13464.

IL-22: Highly-durable low-temperature catalysis driven by uni-sized Pt clusters supported on SiC substrate

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It has been discovered that electrons are accumulated at the sub-nano interface between a Pt cluster and a Si substrate surface, Pt_N/Si,[1] owing to strong interaction between Pt and Si.[2] This enables low-temperature splitting of an O_2 molecule, leading to creation of very active atomic O species at lower temperature by 140 K than a bulk Pt surface.[2] NO splitting occurs also at lower temperature. As a result, unprecedented catalysis in CO oxidation[3] and NO reduction is reachable, as they are initiated and rate-determined by the O_2 and NO splitting, respectively. However, in a way to utilize the unique and high performance of this invention as a practical catalyst, one has to overcome degradation of Pt_N/Si; Si atoms start to dissolve into the Pt cluster at 700 K, so that Pt_N/Si loses its catalytic activity.[2]

It is well known that silicon carbide, SiC, has high chemical and thermal stability, which seems effective to suppress the dissolution of the Si atoms into the Pt cluster. Figure 1 shows an STM image of Pt_{30}/SiC prepared by cluster-impact deposition on a (0001) surface of a 6H-SiC substrate at the collision energy of 90 eV per Pt_{30}^+. Pt_{30} are discernible as protrusions having bi-atomic Pt layers on the Si surface (lower terrace) but no observation on the C surface (higher one). XPS spectra indicate Pt-Si bonding. The CO-oxidation turnover rate on Pt_{60}/SiC at the partial pressures of O_2 and CO of 3×10^{-6} Pa has almost the same temperature dependence as that on Pt_{60}/Si. This high catalytic performance of Pt_N/SiC is maintained even in the repeated catalysis operation as high as 850 K. In conclusion, Pt_N/SiC possesses the low-temperature catalytic activity and are more robust than Pt_N/Si. This study opens the way to a practical catalyst driven by metal clusters supported on a semi-conductor substrate.

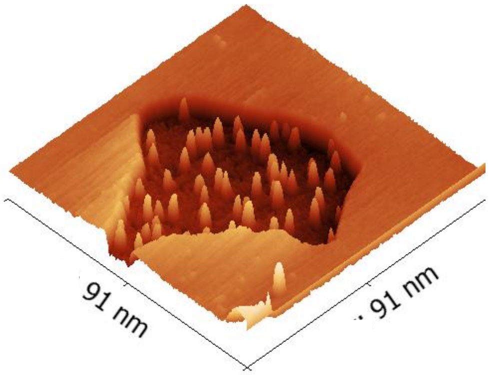

Figure 1: STM image of Pt_{30}/SiC.

Keywords: Pt cluster; SiC; catalysis; CO oxidation; NO reduction

1. N. Fukui and H. Yasumatsu, *J. Chem. Phys.* 151 (2019) 224309.
2. H. Yasumatsu, *Encyclopedia of Interfacial Chemistry: Surface Science and Electrochemistry*, ed. Klaus Wandelt (Editor-in-Chief), Elsevier, Volume 3.2: Clusters and Nanoparticles on Surfaces, pp. 477-489 (2018).
3. H. Yasumatsu, *J. Phys. Chem. C* 124 (2020) 23724.

IL-23: Utilization of CO_2 as feedstock for the synthesis of valuable chemicals

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Carbon dioxide (CO_2) fixation reactions are of paramount interest in the context of uncontrolled release of greenhouse gases and its environmental consequences. Furthermore, these are cost-effective and green organic synthesis as CO_2 is a nontoxic, cheap and abundant renewable C1 source.[1] CO_2 molecules can be made reactive in the presence of suitable catalytic surfaces and it is used as a source of carbon and oxygen for the synthesis of a wide range of value added fine chemicals. Some specific metals (like Ni, Zn, Ag, Pd etc.) as well as reactive functional groups when supported over high surface area porous nanomaterials showed good catalytic activity in the CO_2 fixation reactions. Since there is a wide scope on the types of organic reactions (synthesis of methanol, formic acid, methane, urea, esters, dimethyl ether, dimethyl carbonate, cyclic carbonates, carbamates, carboxylation of alkenes/alkynes, epoxidation of olefins, N-formylation, benzyl formates etc.)[2-6] as well as types of catalytic sites, which can catalyze these CO_2 fixation reactions, these catalytic reactions have huge potential to be explored for the years to come. These reactions are not only environmentally demanding but economic processes also due to the abundance of CO_2 in atmosphere and its low cost as feedstock. In this talk, I will discuss several heterogeneous catalysts based on porous nanomaterials that can be utilized in these CO_2 utilization reactions with the special emphasis of the impact of nanoscale dimensions in catalysis.

References:

1. C. Maeda, Y. Miyazaki and T. Ema, Catal. Sci. Technol. 2014, 4, 1482.
2. S. Bhunia, R. A. Molla, V. Kumari, S. M. Islam and A. Bhaumik, Chem. Commun. 2015, 51, 15732.
3. Q. Liu, L. P. Wu, R. Jackstell and M. Beller, Nature. Commun. 2015, 6, 5933.
4. S. Chongdar, S. Bhattacharjee, S. Azad, R. Bal, A. Bhaumik, Mol. Catal. 2021, 516, 111978.
5. S. Chongdar, S. Bhattacharjee, S. A, S. Samui, S. Dutta, R. Bal, A. Bhaumik, ACS Appl. Mater. Interfaces 2021, 13, 40157.
6. S. Chatterjee, S. Das, P. Bhanja, E. S. Erakulan, R.Thapa, S. Ruidas, S. Chongdar, S. Ray, A. Bhaumik, *J. CO_2 Util.* **2022**, *55*, 101843.

IL-25: Role of intrinsic C-vacancies in CH_4 activation and C-C coupling: The case of Ti_2C

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Activation of methane, the main component in natural gas, and its conversion to useful products is an important chemical process because methane is not only one of the most important feedstocks for fuels and chemicals but also is one of the leading contributors to global warming. However, presence of strong C-H bonds and absence of any dipole or quadrupole moments in methane makes C-H bond scission difficult making the molecule inert.

Transition metal carbides are used both as support and catalysts for different class of reactions. These materials are prone to defects; C vacancies is particular. These vacancies affect the electronic properties that in turn alter their catalytic activity. The vacancies can be either detrimental or benign to the catalytic process. Non-stoichiometric Ti_2C has lines of C-vacancies. In this work, using first-principles density functional theory-based calculations, we have explored the most stable (100) surface of non-stoichiometric Ti_2C as a plausible catalyst for methane activation. We find that these C-vacancies act as reaction centers. Our results show that while cleavage of the first three C-H bonds has very low barriers, the last C-H bond activation has a significantly large barrier. Further, our studies on the feasibility of formation of C_2 products like ethane, ethylene and acetylene shows that these reactions are associated with large activation barriers, which suggest that C-C coupling reactions are not feasible on this surface. The above observation can be attributed to the presence of these C-vacancy lines on the surface. Further, taking into account both the reactions, our results suggests that the presence of such a substantial amount of C-vacancies on the surface would result into formation of large amount of CH and C species bound to the surface, thereby blocking the reaction sites and deactivating the catalyst. From our studies we anticipate that other non-stoichiometric TiC surfaces with lower concentration of C-vacancies can be explored as catalysts for methane activation and C-C coupling reactions.

References:

1. CH4 Activation and C-C coupling on Ti2C(100) Surface in presence of intrinsic C-vacancies: Is excess good?, N. Kuriakose, U. Mondal and P. Ghosh, J. Mater. Chem. A, 9 23703 (2021).

2. CO2 Capture, Activation and Dissociation on Ti2C Surface and Ti2C MXene: Role of Surface Structure, A. Mohan T, N. Kuriakose, K. Mondal, and P. Ghosh, Phys. Chem. Chem. Phys., 22, 14599 (2020).

IL-26: CO_2 reduction and N_2 fixation on transition-metal-doped MIL-88A (Fe)

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Efficient transfer of charges at the interface of transition-metal and semiconductor can improve efficiency of photocatalyst. Herein, we examined photoactivity of Mn and Zn-doped MIL-88A for CO_2 reduction and N_2 fixation by water under UV-visible irradiation and ambient conditions. Gaseous-phase photo-reduction of CO_2 generated CO, H_2, and CH_4. Apparent quantum yield of Zn-MIL-88A was found to be 2.16-folds higher than that of pristine MIL-88A catalyst. Also, the highest NH_4^+ generation rate $(300 \mu mol g^{-1} h^{-1})$ was for Zn-MIL-88A catalyst. Dissecting the underlying mechanism discloses that electrons efficiently transferred from doped transition-metals to the Fe-O cluster of MIL-88A. The hydrophilic surface of the tested catalysts in a tri-phase photocatalyst system led the process to be controlled by mass-transport; which governed the product distribution and limited the kinetics of the process. Experimental results also unveil that the addition of transition metals improved stability, charge-separation, and efficiency of the resulting photocatalysts.

Keywords: Interface; charge-separation; apparent quantum yield; Diffusivity.

IL-27: Rationally designed Intermetallic as Efficient Catalysts for the Selective Conversion of CO_2 to Methanol at Low Energy Input

Dr. Sebastian C. Peter,
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Two most imminent scientific and technological problems that the mankind is facing now, is that of energy and climate. The energy production and utilization in modern society is mostly based on the combustion of carbonaceous fuels like coal, petroleum and natural gas the combustion of which produces CO_2, which alters earth's carbon cycle. 30 billion of tons of CO_2 per year get emitted globally as waste from the carbonaceous fuel burning and industrial sector, which if converted to valuable chemicals have the potential to change the economy of the world. We, in our lab are trying to address both issues and are keen upon translating our innovative technologies from the lab to the industrial and commercial scale. We are capturing CO_2 from industrial flue stream (of any composition) and thermo- catalytically converting it to value added chemicals/fuels such as methanol, carbon-monoxide, methane, dimethyl ether, C2-C5 & C5-C11 gasoline hydrocarbons. Catalyst design is at the heart of all these technologies and we have developed customized catalyst systems for targeted product conversions as per the need of different industries.

In this talk, I will discuss the discovery of two classical intermetallics as efficient catalysts for the conversion of CO_2 to methanol thermochemically and electrochemically using low pressure and low potential, respectively. In the first one, the optimized reaction conditions in the thermochemical pathway favoured the in-situ transformation of Ni_7In_3 to Ni_3In, which favored the conversion of CO_2 to methanol at extreme low pressure. This ordered arrangement of atoms with the isolation of the active site nickel and electronegativity difference between Ni and In are attributed to shift the mechanism towards methanol compared to methane in the case of Ni/SBA-15. The new material favored the conversion of CO_2 to methanol at lower pressure (20 bar) compared to the typical higher pressure (50-100 bar) operation. In the second example, the pseudo two dimensional $CuGa_2$ favoured the selective dissolution of Ga in operando condition favoured the skin layer of oxides of gallium, which enhances the conversion of CO_2 to methanol with record Faradaic efficiency (80%) at extreme low potential. The mechanistic pathway of both processes have been explained by various in-situ (DRIFTS, IR, XAFS), ex-situ (XPS, XRD, IR, XAFS) and theoretical (DFT calculation) studies.

References:

1. Peter, S. C. *ACS Energy Lett*. 2018, *3*, 1557-1561.
2. Roy, S.; Cherevotan, A.; Peter, S. C. *ACS Energy Lett.* 2018, *3*, 1938-1966.
3. Cherevotan, A.; Raj, J.; Dheer, L.; Roy, S.; Sarkar, S.; Das, R.; Vinod, C. P.; Xu, S.; Wells, P.; Waghmare, U. V.; Peter, S. C. *ACS Energy Lett.*, 2021, *6*, 509-516.
4. Bagchi, D.; Raj, J.; Singh, A. K.; Cherevotan, A.; Roy, S.; Manoj, K. S.; Vinod, C. P.; Peter, S. C. *Adv. Mater.* 2022, DOI: 10.1002/adma.202109426.

IL-28: Manifestation and Improvement of Thermoelectric Performance in strain engineered 2D Materials

Prof. G. P. Das
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To meet the rapidly increasing energy demand, renewable and non-conventional energy sources are now in high demand. Thermoelectric generators which can convert thermal energy into electrical energy and vice-versa, have drawn a lot of attention as a possible renewable energy source. In recent years, 2D materials have emerged as a potential thermoelectric material owing to its intrinsically high charge carrier mobility and low thermal conductivity. Among the 2D materials, various layered transition metal chalcogenides and oxides (such as MoS_2, WS_2, ZnO, SnTe, ZnTe etc.) have triggered significant interest in the field of thermoelectric materials due to their high energy conversion efficiency (ZT). Despite the wide research interest and investigation, 2D materials are yet to match the efficiency criteria to become useful in practice. A lot of efforts have been made to improve the thermoelectric performance of 2D materials either by enhancing the Seebeck coefficient and electrical conductivity and/or by reducing the thermal conductivity. Various approaches have been adopted to serve the purpose such as, doping, alloying, forming heterostructures, defect engineering and strain engineering. Herein, we have explored the significance of strain engineering in enhancing the thermoelectric performance of various 2D materials with particular focus on monolayer (ML) ZnO and some TMDCs. Strain engineering is advantageous over the other approaches as it offers reversibility and tunability, unlike via other routes. A significantly enhanced thermoelectric performance is achieved in monolayer MoS_2 and ZnO under the application of in-plane as well as isotropic strains. Strain engineering has been identified as an efficient tool to shift the electronic and phononic bands in energy and frequency, respectively. Strain-induced electronic band convergence and large reduction in lattice thermal conductivity acts in concert to improve the thermoelectric performance of ML-ZnO and MoS_2. The comparatively easier approach and higher effectiveness makes strain engineering an attractive option to fabricate thermoelectric nano-devices using 2D materials.

IL-29:

Aftab Alam

IL-30: Theoretical insights on critical factors that influence the performance of organic solar cells

Mahesh Kumar Ravva,
Department of Chemistry, SRM University – AP, Andhra Pradesh

The design and development of several new high-performing non-fullerene acceptors (NFAs) improved the power of conversion efficiency of organic solar cells. However, the photovoltaic performance is still lower than the commercial inorganic solar cells. In this presentation, we show how the current architecture of NFA limits the performance of organic solar cells. Our results indicate design and choosing the right combination of functional units in NFAs would be an effective way further to improve the power conversion efficiencies of organic solar cells.

IL-31: Discovering unconventional trends in thermal and electronic transport in nanomaterials with defects from first principles

Dr. Ankita Katre,
S P Pune University, Pune, India.

Nanomaterials consist of different kinds of intrinsic and extrinsic defects, that crucially govern electronic and thermal transport properties interesting for cutting edge technologies like thermoelectric, thermal barrier coating, nanoelectronics, LEDs etc. Predictive modelling and developing profound understanding of these transport properties in defective materials is thus fundamentally critical for further advancements, that has remained a challenge to date. With our ab initio study, we unravel novel trends in the electrical and thermal transport properties of technologically interesting materials. We have recently investigated enhanced electrical transport in the nanoflakes of SnSe, a well-known thermoelectric material, by understanding the role of different electron scattering mechanisms [1]. Similarly, novel trends in thermal transport of materials are uncovered too. We find 'vacancy site independence' in transition metal diborides, a class of multifunctional materials interesting for thermal barrier coating applications [2]. Our findings challenge the conventional understanding of larger impact from bigger atom vacancies on material properties. The calculations are performed within an ab initio approach based on Green's function formalism implemented in almaBTE package [3,5] (co-developer). We have shown excellent agreement of thermal conductivities for various materials with experiments [4,5,6,7], and found unique defect behaviours such as 'resonant phonon scattering' for BC substitutional defect in cubic SiC caused by broken structural symmetry around boron defect [5]. Furthermore, I have recently worked on simplified analytical models of defect-phonon scattering [4]. In my talk, I will elaborate on some of these interesting findings and their implications on materials designing and characterization, along with a brief introduction to the ab initio Green's function approach for defects.

References:

[1] Mandava et al., A. Katre*, N. Sonatthi, Nanotechnology, 33, 15, 1557710 (2021)
[2] V. Sonar, R. Dehankar, Vijayalakshmi K. P., A. Katre* (communicated, 2022)
[3] Carrete, Vermeersch, Katre et al., Computational Physics Communications, 220C, 351 (2017)
[4] Gurunathan et al., A. Katre, G. J. Snyder, Physical Review A, 13, 034011 (2020)
[5] Katre* et al., Physical Review Letters, 119, 075902 (2017)
[6] Katre* et al., Physical Review Materials (R), 2, 050602 (2018) [7] Katre* et al., Journal of Materials Chemistry A, 4, 15940 (2016)

IL-32: Diffusion of H on Pt (111): The Effects of Atomic Resonant Tunneling

Dr. Yong Yang,
Chinese Academy of Sciences, China.

The quantum motions of hydrogen (H) atoms play an important role in the properties and functionalities of condensed phase materials. In this talk, I will report on the latest progress of our group on this topic. Using the transfer matrix method and first-principles calculations, we study the quantum motions of H atoms by numerically calculating the quantum probability of H transferring across a number of model potentials and the surface potential fields of Pt(111). Atomic resonant tunneling (ART) is demonstrated along a number of diffusion pathways. Owing to resonant tunneling, anomalous rate of transfer is predicted for H diffusion along certain path at low temperatures. The role of nuclear quantum effects (NQEs) on the surface reactions involving H is investigated, by analyzing the probabilities of barrier-crossing. The effective barrier is significantly reduced due to quantum tunneling, and decreases monotonically with temperature within a certain region. For barrier-crossing processes where the Van’t Hoff-Arrhenius type relation applies, we show the existence of a nonzero low-temperature limit of rate constant, which indicates nontrivial activities of H-involved reactions at cryogenic conditions.

References:

[1] C. Bi and Yong Yang, Atomic Resonant Tunneling in the Surface Diffusion of H Atoms on Pt(111). *Journal of Physical Chemistry C* 125, 464-480 (2021).

[2] C. Bi, Q. Chen, W. Li and Yong Yang, Quantum nature of proton transferring across one-dimensional potential fields. *Chinese Physics B* 30, 046601 (2021).

IL-33: ***Recent Advances in Pentagon-Based 2D Materials***

Prof. Qian Wang
Peking University

IL-34: Theoretical DFT Study on Metal-Organic Frameworks for Hydrogen Storage

Prof. Nurbosyn U. Zhanpeisov,
Tohoku University, Japan.

The cluster approach has been applied to mimic metal-organic framework (MOF) structures formed by 1,4-benzenedicarboxylate linkers and metal cation (or metal oxide) connectors. The geometry optimizations have been carried out at B3LYP/6-31G* level followed by frequency calculations. We have shown that the replacement of OBe_4^{6+} connectors with OMg_4^{6+} (or OZn_4^{6+}) ones leads to an increase in both the unit-cell sizes and basicity of oxide sites making them more potential for molecular hydrogen storage applications. Within the selected secondary building units (larger cluster models), the above replacement does not lead to an alteration on conduction and valence bands as well as in the resulting bandgap values. Bottleneck point of these structures is due to the presence of the so-called “central fourfold coordinated” tetrahedral oxide anion site. It can be efficiently removed via replacement to “distorted cubic core” by introducing $ZnTi_3O_4^{6+}$ (or $MgTi_3O_4^{6+}$) connectors which can be further replaced by $MgSi_3O_4^{6+}$ (or $Al_2Si_2O_4^{6+}$) units. The all threefold coordinated O_{3C} sites formed act as potential adsorption sites for incoming hydrogen molecules. Two-layer ONIOM (MP2/6-31G* : HF/3-21G) calculations have shown that the binding energies of molecular hydrogen lie within 5.5 and 5.3 kJ/mol for the MOF structures with $MgTi_3O_4^{6+}$ and $MgSi_3O_4^{6+}$ connectors, respectively.

Keywords: MOF Structures; B3LYP/6-31G*; ONIOM (MP2/6-31G* : HF/3-21G) calculations; Molecular Hydrogen Adsorption

IL-35: High-Entropy Transition metal oxides

Prof Keivan Esfarzani,
University of virginia,USA.

We present our results on the statistics of distortions in high-entropy transition metal oxides MgCoNiCuZnO5. Molecular dynamics in a supercell have revealed that the amount of distortions in these alloys is relatively large, on the order of 7-10% of the lattice parameter. It was found that distortions increase with temperature. This could strongly affect their thermal properties. We propose control of distortions by changing the stoichiometry of the transition metal elements.

IL-36: 3d-transition-metal-based HEAs by high-throughput sampling based on first-principles calculations

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

To understand structure-property relationship of high-entropy alloys (HEAs), it is important to clarify microscopic ordering mechanism that determines their crystal structures. CrFeCoNi is the most famous ordered phase, but there has been no systematic study for transition-metal HEAs so far. In this work, we systematically considered equiatomic quaternary alloys consisting of four out of Cr, Mn, Fe, Co, Ni, and Cu as constituent elements. Our high-throughput first-principles simulations sampled and evaluated a large number of atomic configurations of their ordered $L1_2$ and $D0_{22}$ phases as well as random solid solution (RSS) phases, thereby investigating their energetics dependence. We found that the valence electron concentration (VEC) and temperature considering the configurational entropy term are the key factor to determine the phase stability of the HEAs at finite temperature: depending on their VEC values, ordered phases are energetically more favorable than RSSs and some $D0_{22}$ ordered phases are energetically more stable than $L1_2$ phases. The results indicate that the phase stability is realized by an order–disorder “competitive cooperation”, i.e., cooperation between “one magnetically ordered atomic configuration gaining enthalpy” and “the other three random atomic configurations gaining entropy”. This work was supported by Bilateral Collaboration Program through the National Research Foundation of Korea (NRF) funded by the Ministry of Science and ICT (Grant No. 2021K2A9A2A0700009311). This study was supported by the computational resources of the HPCI system (Project ID: hp190014, hp190059, hp200040, hp210019), the JHPCN system (Project ID: jh190019), Institute for Materials Research, Tohoku University (Proposal No. 19S0501, 20S0505, 202012-SCKXX- 0506), JAIST, and NIMS.

Reference: https://arxiv.org/abs/2110.02587

Keywords: high-entropy alloys, ordered phases, enthalpy driven, entropy driven, first-principles calculations

IL-37: Effect of doping on electronic structure and magnetostriction in FeGa alloys

Prof. Talgat M. Inerbaev,
Novosibirsk state university,Russia.

The electronic structure of doped FeGa alloy is investigated theoretically using methods of the density functional theory. The work aims to uncover the difference in the material's magnetostrictive properties when doping with transition metals or La as the simplest representative of rare-earth elements. The effect understudy was investigated by considering the change in two features of the electronic structure caused by doping: the density of *d*-states on Fe atoms and the nature of the Fe-Fe bonding near the doping atom. The transition metal atoms are surrounded by Fe atoms with a low-density *d*-states, eliminating the doping effect. The interatomic bonds of transition metals with the nearest Fe atoms have an antibonding character, while bonds between Fe atoms of the first and second coordination spheres are more binding than in an undoped alloy. This effect leads to magnetostriction decrease. In the La-doped alloy, the opposite picture is found. An increase in magnetostriction should occur due to the enhancement of the antibonding character of bonds between Fe atoms in the first and second coordination spheres of the dopant. For a detailed study of the effect of doping on the electronic structure of the FeGa alloy, we investigated the Fe_3Ga compound of the $D0_3$ structure. The $D0_3$ crystal lattice contains Fe atoms of two types with different local coordination. The study of the effect of doping on the density of *d*-states of Fe atoms and the change in the electronic band structure explains why various dopants have other effects magnetostriction of FeGa alloys.

Keywords: FeGa alloy; magnetostriction; doping; computer modeling

IL-38: Integrated first-principles approach for modelling microstructure evolution in multi-component alloys under irradiation

Prof. Duc Nguyen-Manh,
United Kingdom Atomic Energy Authority, Oxfordshire, United Kingdom.

Phase stability of multi-component alloys under non-equilibrium irradiation conditions represents one of most challenging issues not only in computational materials science but also in developing radiation-resistance engineering components within nuclear fusion reactors. Recently, a body-centred cubic tungsten-based refractory high-entropy alloys (HEAs) with reduced activation and outstanding radiation resistance has been developed for plasma-facing materials in future fusion power plants.

To address these challenges, a new integrated modelling approach based on first-principles formulation of constrained thermodynamic formalism has been developed to model multi-component alloy system under irradiation for which radiation defect clusters are being incorporated into effective cluster expansion Hamiltonian model. In combination with Monte-Carlo simulations, the methods alloys to predict microstructure of complex materials as a function of alloy composition at arbitrary irradiated temperature. Most recently, we have extended the current approach in developing an efficient scheme of machine-learning potentials (MLPs) by using thousands of DFT data from the representative structures of alloys, defects with applied strains and AIMD simulations in both solid and liquid phases. configurations under applied an extensive considered as the additional elements in the system. The developed MLPs are shown to produce an excellent accuracy in term of energies, forces and stresses for benchmarking a case of study for W-based HEAs. The newly developed MLPs provide the tool for performing large scale molecular-dynamic simulations and predicting microstructure evolution in complex materials under strong neutron irradiation.

Keywords: first-principles modelling, composition dependence of HEAs, short-range order, neutron irradiation, machine-learning potentials.

IL-39: Designing features and understanding why they work.

Dr. Kavita Joshi,
Physical and Materials Chemistry Division,
CSIR-NCL, Pune,India.

Machine learning (ML) is used extensively in last couple of years to discover materials with desired properties or to uncover hidden correlations. One of the crucial factors in successfully employing ML based models is designing features and understanding why they work. In this talk, I will present the recent work carried out in my group. We employed ML based model with an aim to predict bondlength activation and adsorption energies of various molecules on different transition metal surfaces. Our investigations bring out missing one to one correlation between adsorption energies and corresponding bondlength activation. We also provide rationale as to why the model works.

Keywords: Machine Learning, DFT, Catalyst

IL-40: Exploring Chemical and Physical Space of Carbohydrates by Quantum Chemistry assisted by Machine Learning Methods

Prof. Jer-Lai Kuo,
Institute of Atomic and Molecular Sciences, Academia Sinica,Taiwan.

The four basic categories of molecules involved in creating life are nucleic acids, proteins, carbohydrates, and lipids. To understand their physical chemical and biological properties, it is necessary to obtain more information on their structure. However, owing to the large number of isomers for a given chemical formula of carbohydrates, the development of robus analytical methods to obtain the structure of carbohydrates remains a challenge. In the last 10 years, we have developed *ab initio* structural searching and anharmonic algorithms to search for stable conformers of molecular systems – that is the physical space of carbohydrate. Recently, mass spectrometry (MS) in gas phase under Collision-induced dissociation (CID) has been applied in the structural analysis of carbohydrates[1-6]. To understand the underlying reaction mechanism, we need to explore transition states – that is the chemical space of carbohydrate. In this talk, I will present our recent effort in using deep learning neutral network to speed up the exploration of both the physical and chemical space of carbohydrates with quantum chemistry accuracy.

References:

1. J-L Chen, H-S Ngua, P-J Hsu, S-T Tsai, C-Y Liew, *J-L Kuo*, W-P Hu, and C-K Ni*, Phys. Chem. Chem. Phys.* 19, 15454-15462 (2017)
2. H. Huynh, H. T. Phan, P-J Hsu, J-L Chen, H-S Nguan, S-T Tsai, T. Roongcharoen, C. Y. Liew, C-K Ni, *J-L Kuo*, *Phys. Chem. Chem. Phys.*, 20, 19614-19624 (2018)
3. C-c Chiu, S-T Tsai, P-J Hsu, H. Huynh, J-L Chen, H. T. Phan, S-P Huang, H-Y Lin C-Y Liew, , *J-L Kuo*, C-K Ni*, J. Phys. Chem*, A 123, 3441-3453 (2019)
4. C-c Chiu, H. Huynh, S-T Tsai, H-Y Lin, P-J Hsu, H. T. Phan, A. Karumanthra, H. Thompson, Y-C Lee, *J-L Kuo*, C-K Ni*, J. Phys. Chem*, A 123, 6683-6700 (2019)
5. C-c Chiu, C-K Lin, *J-L Kuo*, *Phys. Chem. Chem. Phys.*, 22, 6928 (2020)
6. H-S Nguan, S-T Tsai, J-L Chen, P-J Hsu, *J-L Kuo*, C-K Ni*, Phys. Chem. Chem. Phys.*, 23, 3485 (2021)

Keywords: Carbohydrate; Quantum Chemistry; Neural Network

IL-41: Computational materials design from materials simulations to informatics

Prof. Kenta Hongo,
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Materials Informatics (MI) [1] has attracted enormous attention in materials science. About a decade ago, computational material design relied only on materials simulations, considering a small search space limited to tens to hundreds of compounds. On the other hand, MI such as high-throughput virtual screening approaches based on machine learning techniques expands its search space into that in the order of hundred thousand of compounds. In particular, ab initio simulations based on density functional theory (DFT) have been widely used to generate various materials property data. Although DFT succeeds in describing most property predictions, but it fails in some cases (e.g., strongly correlated systems, noncovalent systems, etc). One of the most practical approaches to circumventing the DFT failures is quantum Monte Carlo (QMC), especially diffusion Monte Carlo (DMC). QMC stochastically solves the many-body Schrödinger equation with a good balance between accuracy and computational cost, and hence is quite suitable for recent massively parallel computers because of its high parallel efficiency. For the next-generation exascale supercomputers, QMC can be used as one of the next generation "data generation engines" in the "ab initio MI". In this talk, I will present a brief introduction to MI followed by our recent achievement [2-7] as well as materials simulations [8,9].

Keywords: Ab initio simulations, Materials informatics, Machine learning, Bayesian Inference

References:

1. Gomez-Bombarelli, R.; et al., Nat. Mater. 2016, 15, 1120-1127.
2. Ikebata, H.; et al., R. J. Comput. Aided Mol. Des. 2017, 31, 379-391.
3. Wu, S.; et al., npj Comput. Mater. 2019, 5, 66:1-11.
4. Yoshida, T.; et al., ACS Omega 2020, 5, 13403-13408.
5. Yoshida, T.; et al., ACS Appl. Nano Mater. 2021, 4, 1932-1939.
6. Utimula, K.; et al. Adv. Theory Simul. 2020, 3, 2000039:1-9.
7. Peng, S.; et al. Chem. Mater. 2021, 33, 9501-9507.
8. Kato, D.; Hongo, K.; et al., J. Am. Chem. Soc. 2017, 139, 18725-18731. 9. Hongo, K.; et al., J. Phys. Chem. Lett. 2010, 1, 1789-1794.

IL-42: Internal Data driven Catalysis Research- High throughput experiments and high throughput simulations

Dr. Sandip De, BASF SE, Germany.

In this talk I aim to provide a glimpse into the fast paced industrial catalysis development research at BASF. Through some examples, I will discuss how we are combining high throughput experiments with high throughput simulations and how the data-science and machine learning methods are helping us find unexpected shortcuts in the complex world of heterogeneous catalysis. I will end the talk with some perspectives and challenges in the present "data driven" scientific research paradigm. References 1. Learning Design Rules for Selective Oxidation Catalysts from High-Throughput Experimentation and Artificial Intelligence, ACS Catal. 2022, 12, 4, 2223–2232 2. Comparing molecules and solids across structural and alchemical space, Phys. Chem. Chem. Phys., 2016,18, 13754-13769 3. Machine learning unifies the modeling of materials and molecules,SCIENCE ADVANCES ,2017,Vol 3, Issue 12

IL-43: Charged Defects in TiO_2 Anatase: A Comparative Study of Hybrid DFT, GW and BSE to Explore Optical Properties

Dr. Saswata Bhattacharya,
Indian Institute of Technology, Delhi,India.

Titanium dioxide (TiO_2) anatase is one of the most abundant, functionally versatile oxide materials, with applications in the field of opto-electronic devices and solar cell conversion efficiency. However, owing to its large bandgap (3.2 eV), the photo-absorption efficiency is limited only in the UV region. Doping-mediated modulation is one of the most pragmatic approaches in the pursuit to improve the photocatalytic and solar energy conversion efficiencies of TiO_2. We report here using state-of-the-art hybrid density functional and *ab initio* atomistic thermodynamics, the thermodynamic (meta-) stability of different non-metal dopants X (X= N, C, S, Se) as a function of charge state at realistic temperature and pressure. We have obtained that charged defects (mainly substitution/interstitial type) play an important role in providing enhanced stability, by carefully analyzing the individual effect of bond-making/breaking and charge carrier trapping energies. Knowing the most stable defects, we aim an accurate theoretical estimation of the optical properties of doped TiO_2 for both scientific and practical interest. To do this, we have used many body perturbation theory viz. one particle Green's function (GW) method and higher order Green's function techniques (that includes the effect of excitons) Bethe-Salpeter Equation (BSE). The calculated quasiparticle excitation energies of pristine anatase TiO_2 are in good agreement with available photoemission and inverse photo-emission results. Further, our calculations reveal the highly anisotropic nature of the doped TiO_2. The n-type doped TiO_2 is optically active in both x, z direction, whereas the p-type doped TiO_2 is optically inactive along z-direction. The most evident hallmark of the doped system is the appearance of absorption peaks at low energy below 3 eV, to give rise visible-light absorption.

IL-44: Engineering multifunctionality at oxide interfaces by structural mode coupling

Dr. Saurabh Ghosh
SRM Institute of Science Technology, Chennai, India.

Mode coupling in real materials not only drives structural phase transition but also drives functional properties into the low symmetry phase. The ABO3 perovskite oxides are among the most studied systems owing to their functional properties such as ferroelectricity, weak ferromagnetism, linear magnetoelectricity and many other, primarily driven by structural distortions [1–3]. Here, we employed first-principles density functional theory calculations guided by group-theoretical analysis and demonstrated the control of insulator-metal-insulator transition, polarization and two sublattice magnetization in (LaFeO3)1/(CaFeO3)1 superlattice via. multi structural mode coupling i.e., 'multimode coupling'. We have discovered a polar Atype charge disproportionation mode, QACD (analogous to the A-type antiferromagnetic ordering), and found that it couples with the trilinear coupling, QTri mode (common in Pnma perovskite oxides and involves three structural modes), and lowers the symmetry further. By tuning the strength of the coupling between the participating modes, the polar metallic phase, polar zero bandgap semiconducting, and polar insulating phases can be obtained. The QTri mode switches the polarization direction, whereas, QACD can trigger insulator-metal-insulator transition along with the polarization switching. The mechanism is true for any transition metal superlattices constituted with Pnma building blocks and with partially filled eg or t2g electron(s) at the transition metal sites [4].

References:

[1] N. A. Benedek and C. J. Fennie, Phys. Rev. Lett. 106, 107204 (2011).
[2] S. Ghosh, H. Das, and C. J. Fennie, Phys. Rev. B 92, 184112 (2015).
[3]S. Ghosh, A. Y. Borisevich, and S. T. Pantelides, Phys. Rev. Lett. 119, 177603 (2017).
[4] M. Shaikh, M. Karmakar, and S. Ghosh, Physical Review B 101, 054101 (2020).
[5] M. Shaikh and S.Ghosh (submitted, in peer review)

IL-45: Large-Scale Molecular Dynamics Simulations on Chemical-Reaction-Induced Wear Processes of Diamond-like Carbon Films

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In recent years, due to strong demands for energy saving and carbon neutrality, maximizing energy utilization efficiency in automobiles, airplanes, industrial robots, information equipment, etc. is required. To realize the above tasks, super-low friction and super-low wear technologies have become urgent social issues. Specifically, about 20 % of total energy loss in automobiles is due to friction and about 75 % of causes of the mechanical equipment failure is due to friction-induced wear. Since urgent measures are required for the above problems, it is desired to establish theoretical design technologies for super-low friction and super-low wear. Many friction simulations have been done by molecular dynamics approaches, however, the establishment of wear process simulation technologies are challenges for next-generation because the chemical reaction dynamics in large-scale model during the friction processes should be treated for elucidating the wear processes and mechanisms. Therefore, in the present study, we employed our supercomputer "MASAMUNE-IMR" and in-house large-scale molecular dynamics code to simulate both chemical-reaction-induced and mechanical-force induced wear processes. The detailed outcomes of our chemical-reaction-induced and mechanical-force induced wear simulations of diamond-like carbon films will be presented in the conference [1,2].

[1] Y. Wang, N. Yamada, J. Xu, J. Zhang, Q. Chen, Y. Ootani, Y. Higuchi, N. Ozawa, M.-I. De Barros Bouchet, J. M. Martin, S. Mori, K. Adachi, and M. Kubo, Sci. Adv., 5 (2019) eaax9301.
[2] Y. Wang, J. Xu, Y. Ootani, N. Ozawa, K. Adachi, and M. Kubo, Adv. Sci. 8 (2021) 2002827.

Keywords: Large-Scale Molecular Dynamics Simulations, Wear, Diamond-like Carbon, Chemical Reaction

IL-46: Structural deformations in MXenes: Charge-density waves and electrides

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MXenes are 2D materials composed of carbon or nitrogen (X) layers sandwiched between metal (M) layers, and terminated by oxygen, fluorine, or some functional group (T). The central X layer usually is hexagonal, and most of MXenes are metallic. Focusing on carbide MXenes with formula M_2CT_2, we first device a simple counting rule to determine basic properties of MXenes (metallic, insulator, magnetic, or non-magnetic etc.) based on formal charges [1]. We then investigate some special cases, where charge disproportionation brings about structural deformations that break the hexagonal symmetry of the central X layer, manifested by charge density waves and electride properties [2].

[1] S. Bae, J-G. Kang, M. Khazaei, K. Ohno, Y-H. Kim, M. J. Han, K. J. Chang, and H. Raebiger, Materials Today Advances 9, 100118 (2021).
[2] S. Bae, W. Espinoza-Garcia, J-G. Kang, N. Egawa, J. Lee, K. Kuwahata, M. Khazaei, K. Ohno, Y-H. Kim, M. J. Han, H. Hosono, G. M. Dalpian, and H. Raebiger, Advanced Functional Materials 31, 2100009 (2021).

Keywords: MXene, electride, charge density wave

IL-47: Suppression of Oxidation in Perovskites CH3NH3PbI3 by Lithium-ion Endohedral Fullerenes Li+@C60

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Halide perovskites have attracted a lot attention because of their potential for realizing highefficient low-cost photovoltaics. Among the halide perovskites, methyl-ammonium lead triiodide CH3NH3PbI3 is one of the most widely studied compounds. One of the issue encounters in the practical application of CH3NH3PbI3 perovskites is the poor stability. When the perovskites are exposed to moisture, oxygen, thermal and sunlight, it degrades easily, leading to the declination of the device performance. Recently, Jeon et al. [Angewandte Chem. 2018, 57, 4607] demonstrated that air stability of more than 1000 hours under light illumination can be achieved in CH3NH3PbI3 perovskite solar cells when Li+ is replaced by Li+@C60 in a dopant material used in the p-type donor layer. In order to understand the role of Li+@C60 molecule in the hole transporting materials, we perform first-principles calculations of Li+@C60 adsorbed on CH3NH3PbI3 surface. We construct finite slab models of tetragonal CH3NH3PbI3 (001) surfaces with CH3NH3I terminations and introduced a Li+@C60 molecule on various position of perovskite surface. The Kohn-Sham orbitals and energy eigenvalues of the CH3NH3PbI3/Li+@C60 heterojunction are calculated and discussed. Keywords: CH3NH3PbI3; perovskite solar cells; fullerenes; oxidation

IL-48: Charge Generation in Emerging Non-fullerene Organic Solar Cells

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Organic solar cells (OSC) are one of the emerging PV technologies that are currently investigated as a potential low-cost renewable energy source. Recently, 19 % power conversion efficiency (PCE) is reported for single bulk heterojunction (BHJ) binary OSC and above 20 % for tandem OSCs.[1, 2] To improve further the PCE, the charge generation and extraction should be improved. The minimum energy offset required to ensure efficient charge separation at organic donor-acceptor heterojunctions is a matter of current debate.[3] In this talk, I will be presenting about the charge generation in a series of donor – acceptor bulk heterojunction blends, including the small molecule donor DR3, two high-efficiency donor polymers (PBDB-T-2F, PCE10), and eight different non-fullerene acceptors (NFA), spanning a power conversion efficiency range from <1% to above 15%.[4] In principle, electron affinity (EA) and ionization energy (IE) offsets should control the charge generation equally. However, we demonstrate that despite large EA offsets, the IE offset controls both the exciton quenching and charge separation efficiency, as ultrafast energy transfer from the donor to the acceptor competes with photo-induced electron transfer.[4] This implies that the IE offset cannot be reduced to zero to maximize the V_{OC} as it leads to inefficient exciton quenching and reduced charge separation efficiencies and in turn, to lower device photocurrents and performance.[4] We also extend this study to ternary OSCs and observe the IE offset-driven charge generation.

References:

1.Zheng, Z.; Wang, J.; Bi, P.; Ren, J.; Wang, Y.; Yang, Y.; Liu, X.; Zhang, S.; Hou, J., Tandem Organic Solar Cell with 20.2% Efficiency. *Joule* 2022, *6* (1), 171-184.
2.Cui, Y.; Xu, Y.; Yao, H.; Bi, P.; Hong, L.; Zhang, J.; Zu, Y.; Zhang, T.; Qin, J.; Ren, J.; Chen, Z.; He, C.; Hao, X.; Wei, Z.; Hou, J., Single-Junction Organic Photovoltaic Cell with 19% Efficiency. *Advanced Materials* 2021, *33* (41), 2102420.
3.Wu, J.; Cha, H.; Du, T.; Dong, Y.; Xu, W.; Lin, C.-T.; Durrant, J. R., A Comparison of Charge Carrier Dynamics in Organic and Perovskite Solar Cells. *Advanced Materials* 2022, *34* (2), 2101833.
4.Karuthedath, S.; Gorenflot, J.; Firdaus, Y.; Chaturvedi, N.; De Castro, C. S. P.; Harrison, G. T.; Khan, J. I.; Markina, A.; Balawi, A. H.; Peña, T. A. D.; Liu, W.; Liang, R.-Z.; Sharma, A.; Paleti, S. H. K.; Zhang, W.; Lin, Y.; Alarousu, E.; Anjum, D. H.; Beaujuge, P. M.; De Wolf, S.; McCulloch, I.; Anthopoulos, T. D.; Baran, D.; Andrienko, D.; Laquai, F., Intrinsic efficiency limits in low-bandgap non-fullerene acceptor organic solar cells. *Nature Materials* 2021, *20* (3), 378-384.

IL-49: 2D halide perovskites and rare-earth doping for solar energy and optoelectronic applications

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2D halide perovskites have been attracting great attention in recent years for solar energy applications because of their enhanced stability compared to bulk. In this talk I shall present our recent results on 2D inorganic halide perovskites [1] and the effects of surface ligands on their stability [2]. Replacement of H with F or Cl in the phenyl group of the phenylethyl ammonium (PEA) surface ligands has been found [3] to lead to increased stability of the layers. The manipulation of the ligands leaves the optical properties of the layers mostly unaffected as they arise from the inorganic layers. Further studies have been done on double halide perovskites [4] to avoid toxic Pb. The doping of rare earths such as Eu in these direct band gap semiconductors has been found to be very promising for optoelectronic applications [5,6] in contrast to the well-studied compound semiconductors where strain due to rare-earth doping is a problem.

Acknowledgements: This work has been performed in collaboration with Dr. Anu Bala under the DST projects SR/WOS-A/PM-1042/2015 and SR/WOS-A/PM-53/2019. The calculations have been performed on Magus high performance computing system of Shiv Nadar University.

References

[1] A. Bala, A.K. Deb, V. Kumar, J. Phys. Chem. C **122** (2018) 7464.
[2] A. Bala and V. Kumar, J. Phys. Chem. C **123** (2019) 25176.
[3] A. Bala and V. Kumar, ACS Appl. Energy Materials **4** (2021) 1860, and to be published.
[4] A. Bala and V. Kumar, Phys. Rev. Materials **5** (2021) 095401.
[5] A. Bala and V. Kumar, J. Phys. Chem. C**123** (2019), 6965.
[6] A. Bala and V. Kumar, ACS Appl. Nano Materials **3** (2020) 4437.

IL-50: Ab initio investigations of green cesium tin halide quantum dots for photovoltaic applications

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Lead based hybrid organic inorganic, all inorganic perovskites have been demonstrated to have high photovoltaic (PV) efficiencies and have been actively researched for application in solar cells. However, the toxicity of lead, high electron-hole recombination rates and stability under ambient conditions of such solar cells are of concern. Hence non-toxic, stable, environment friendly materials are of immense interest. Using first principles density functional theory-based simulations, we have investigated ligated CsSnX3 (X=Cl, Br, I) - derived quantum dots to assess their suitability for PV cells. The effect of size and choice of ligand on the stability, highest occupied molecular orbital - lowest unoccupied molecular orbital (HOMO-LUMO) gap, excitonic energies and optical properties were studied. All QDs exhibit good absorption in the useful UV-Vis region of the spectrum and natural transition orbital analysis shows the charge transfer on optical excitation occurs from halide p orbital to Sn p orbital. Larger QDs allow for greater charge separation and lower recombination rates, increasing the PV efficiency. Our work shows that good electronic and optical absorption properties, with appropriate band gaps and wide tunability, make H+ ligated CsSnI3 -- derived QDs promising candidates for PV applications.

IL-51: Electrocatalytic Reduction of NO_3^- to Ultrapure Ammonia on {200} Facet Dominant Cu Nanodendrites: Experiment and DFT study

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Nitrate reduction reaction (NtRR) is considered as a green alternative method for conventional way of NH_3 synthesis (Haber-Bosch process), which is known as high energy consuming and large CO_2 emitting process. Herein, the copper nanodendendrites (Cu NDs) grown along with {200} facet as an efficient NtRR catalyst has been successfully fabricated and investigated. It exhibited high faradaic efficiency of 97% at lower overpotential (-0.3 V vs RHE). In-situ Fouriertransform infrared spectroscopic studies (FT-IR) were carried out to examine and affirm the production of NH_3 from NO_3^- over the surface of Cu NDs. Furthermore, the $^{15}NO_3^-$ isotope labelling method was utilized to confirm the formation of NH_3 from Cu NDs. Both experimental and theoretical studies showed that NtRR on Cu is a facet dependent process. Dissociation of NO bonding is supposed to be the rate determining step as NtRR is a spontaneously reductive and protonation process for all the different facets of Cu. Density functional theory (DFT) calculations reveals that Cu {200} and Cu {220} offer lower activation energy for dissociation of NO compared to that of Cu {111}. The new insights provide by this work will pave the way for better understanding and developing of new electrocatalysts for NtRR. [1] .

Keywords: Cu nanodendendrites, nitrate reduction reaction (NtRR), ammonia synthesis, facet dependent, Cu {200}

Acknowledgement: We thank the NCHC and NTUST for providing massive computing time and financial support. Reference: 1. J. Phys. Chem. Lett. 2021, 12, 8121-8128.: https://doi.org/10.1021/acs.jpclett.1c02236

IL-52: A Manmade Nitrogen Cycle: Electrochemical Nitrogen Reduction Reaction with Nanostructured Catalysts

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As an important chemical product and carbon-free energy carrier, ammonia has a wide range of daily applications in several related fields. The industrial method of producing ammonia employing the Haber-Bosch process (HBP) consumes huge energy and liberates CO_2 into our atmosphere. Therefore, the clean and sustainable electrocatalytic N_2 reduction reaction (NRR) operating under mild conditions has attracted great attention in recent years. Electrocatalytic NH_3 production from nitrogen is one of the alternatives to the HBP for sustainable and distributed NH_3 production, primarily when powered by renewable energy, drastically reducing the carbon footprint in our atmosphere. However, such a process has been hampered by the lack of efficient N_2 reduction electrocatalysts. Besides, NH_3 is considered an ideal hydrogen storage medium due to its relatively high hydrogen content of ~ 17 wt.%. Over the past five years, researchers have explored some effective and promising active centers to boost the adsorption and activation of N_2, combined with some low-dimensional nanomaterial substrates with high specific surface area, abundant exposed active sites, and unique electronic morphology to improve the performance of the NRR. In this lecture, I would discuss a few NRR catalytic systems developed in our laboratory. In addition, the theoretical mechanisms, reaction pathways, and credibility studies of the NRR will be discussed.

IL-53: Exploring single, double, and triple atom catalysts for electroreduction of N2 and CO2 molecules.

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Design of cost effective and efficient catalysts for the reduction of small molecules in green manner remains a great challenge in the 21st century. Recently one to few atoms dispersed on suitable supports have attracted considerable attention due to their enhanced reactivity and catalytic activity towards small molecule activation and reduction. In this talk, I will be talking about our recent research using first principles simulations on the activity of single, double, and triple atom catalysts and the underlying electronic factors for reduction of N2 and CO2 molecules to valuable products.

Keywords: First principles simulations, Single atom catalysts; Small molecule reduction.

Oral Presentation

O-01: Mn3O4 Nano octahedrons embedded in N-doped graphene oxide as potent anode material for Li-ion batteries

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Abstract:

Among various electrical energy storage devices, the lithium-ion batteries are one of the versatile and successful energy storage devices in an integral part of portable electronics to electric vehicles. The study of new strategies and materials are needed to achieve high energy density, good cyclic stability and safer Li-ion technology. In this context, we report highly stable Mn3O4 embedded in N-doped graphene oxide (MNGO) as a potent anode, prepared via facile microwave digested hydrothermal route. The structure, morphology and compositions of the synthesized samples are investigated by Raman, XRD, SEM, HR-TEM and XPS techniques. The electrochemical behaviour of materials are tested as anode materials by Cyclic Voltammetry (CV), Galvanostatic charge-discharge (GCD) and Electrochemical Impedance Spectroscopy (EIS). The performance of MNGO is much enhanced due to its lower charge transfer resistance and faster Li+ ion diffusion compared to the reduced graphene oxide (rGO) and Mn3O4. The MNGO has shown excellent cyclic stability with a reversible capacity of 756 mAh/g (almost equal to calculated capacity 780mAh/g) and high Columbic efficiency (96%).

O-02: Theoretical Insights on Molecular Designing of Hot-Exciton based Thermally Activated Delayed Fluorescence Molecules

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Abstract:

Despite the recent breakthroughs on the TADF process, more research is needed to understand its mechanism and develop rational molecular designs for structures with higher efficiencies and quantum yield. Hot exciton-based TADF materials, like traditional (cold) TADF, can effectively utilize the singlet and triplet excitons, theoretically resulting in 100% IQE. However, in contrast to cold TADF (from low-lying T_1 to S_1), the RISC process in hot TADF occurs from high-lying triplet to singlet excited states (from $T_m(m>1)$ to $S_n(n>1)$). But, designing materials that satisfy conditions for hot exciton formation, such as large triplet spacing in lower states and a tiny singlet-triplet gap in higher states, remains a difficult job. In this study, we explore and analyze the fundamental concepts of molecular design and suggest a design strategy as well as structure-property relationships for hot-TADF molecules. This study could lead to new insights into molecular design approaches for organic materials with many hot exciton channels, which could lead to better exciton utilization.

Keywords: TADF; HLCT; spin orbit coupling; hot-exciton; higher-reverse intersystem crossing

O-03: Capturing excitonic and polaronic effect in lead free double perovskites from many-body perturbation theory

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Abstract:

Lead free all-inorganic alloyed double perovskites with formula $A_2B'B''X_6$ have redefined the photovoltaic research in recent past due to low toxicity, intrinsic thermodynamic stability, and small carrier effective mass. In particular, the double perovskite $Cs_2AgInCl_6$ has been the subject of several studies, revealing excellent environmental stability and promising optoelectronic properties. However, a detailed study on their optical, excitonic, polaronic and transport properties remain unexplored so far. Here, we explore the variation of carrier-lattice interaction and optoelectronic properties of pristine as well as alloyed $Cs_2AgInCl_6$ double perovskites using a combined state-of-the-art many-body perturbation theory (G_0W_0@HSE06) and density functional perturbation theory (DFPT). Our results reveal that in comparison to pristine, the alloyed compounds have longer exciton lifetime, indicating a lower electron-hole recombination in the latter. This also leads to higher quantum yield and conversion efficiency in the alloyed compounds. The phonon scattering is found to limit the charge-carrier mobilities and thus, plays an important role in the development of high-efficiency perovskite photovoltaics. We have also observed dominant carrier-phonon scattering via Frohlich mechanism near room temperature. A significant increase in hole and electron mobilities is noticed on alloyed perovskites in comparison to its pristine counterpart making the former to be more potent in photovoltaic devices.

Keywords: excitonic; polaronic; DFPT; Frohlich

O-04: Origin of Rashba spin-splitting and strain tunability in ferroelectric bulk $CsPbF_3$

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Abstract:

Spin–orbit coupling (SOC) in conjunction with broken inversion symmetry acts as a key ingredient for several intriguing quantum phenomena such as persistent spin textures, topological surface states and Rashba–Dresselhaus (RD) effects. RD splitting has attracted considerable attention owing to its rich physics and vast applications in the rapidly burgeoning field of spintronics. The coexistence of spontaneous polarization and the RD effect in ferroelectric (FE) materials enables the electrical control of spin degrees of freedom. In light of this, we explore the FE lead halide perovskite $CsPbF_3$ as a potential candidate in the field of spintronics by employing state-of-the-art first-principles-based methodologies, viz., density functional theory (DFT) with semilocal and hybrid functional (HSE06) combined with SOC and many-body perturbation theory (G_0W_0). For a deeper understanding of the observed spin splitting, the spin textures are analyzed using the ***k.p*** model Hamiltonian. We find there is no out-of-plane spin component indicating that the Rashba splitting dominates over Dresselhaus splitting. The large value of α_R at conduction band minimum (CBm) shows that the Rashba-type spin-splitting dominates at CBm. We also observe that the strength of Rashba spin splitting can be substantially tuned on application of uniaxial strain (±5%). More interestingly, we notice reversible spin textures by switching the FE polarization in $CsPbF_3$ perovskite, making it potent for perovskite-based spintronic applications.

Keywords: Rashba–Dresselhaus; DFT; ***k.p*** perturbation theory; symmetry

O-05: Exploring Exciton and Polaron Dominated Photophysical Phenomena in Ruddlesden-Popper Phases of Ban+1ZrnS3n+1 (n=1-3) from Many Body Perturbation Theory

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Abstract:

Ruddlesden-Popper (RP) phases of $Ba_{n+1}Zr_nS_{3n+1}$ are an evolving class of chalcogenide perovskites in the field of optoelectronics, especially in solar cells. However, detailed studies regarding its optical, excitonic, polaronic, and transport properties are hitherto unknown. Here, we have explored the excitonic and polaronic effect using several first-principles based methodologies under the framework of Many Body Perturbation Theory. Unlike its bulk counterpart, the optical and excitonic anisotropy are observed in $Ba_{n+1}Zr_nS_{3n+1}$ (n = 1-3) RP phases. As per the Wannier-Mott approach, the ionic contribution to the dielectric constant is important, but it gets decreased on increasing n in $Ba_{n+1}Zr_nS_{3n+1}$. The exciton binding energy is found to be dependent on the presence of large electron-phonon coupling. We further observed maximum charge carrier mobility in the Ba_2ZrS_4 phase. As per our analysis, the optical phonon modes are observed to dominate the acoustic phonon modes, leading to a decrease in polaron mobility on increasing n in $Ba_{n+1}Zr_nS_{3n+1}$ (n = 1-3).

Keywords: Ruddlesden-Popper phases; exciton; polaron

O-06: Computational evaluation of the effect of end-cap group modification on the core groups of non-fullerene acceptors for organic solar cell applications

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Abstract:

Organic solar cells which contain small molecules with acceptor–donor-acceptor (A-D-A) structure as electron acceptors have received a lot of interest. These small molecules (also called non-fullerene acceptors (NFAs)) exhibit broad absorption, a high absorption coefficient, robust electron mobility, and tunable energy levels which makes as a potential acceptor compared to fullerene derivatives. The structural features of A-D-A acceptor molecules can be tuned by altering various donor and acceptor units. The choice of donor and acceptor units dictates the electronic and optical properties of NFAs. The energy level alignment between polymer donor and NFAs is one of the important criteria for efficient charge separation, high open-circuit voltage, and reduce the energy loss. Thus, in this study we aim to design various NFAs which has various combinations of donor and acceptor molecules. The impact of acceptors on electronic and excited state properties of newly designed is studied using state-of-the-art density functional theory (DFT) methods. We also model the interface between polymer donor and NFAs to gain more insights into the exciton dissociation and charge recombination rates. All these results will provide guidelines to design efficient combination of electron-donor and electron-acceptor for higher power conversion efficiencies.

Keywords: fused-ring electron acceptors; organic solar cells; density functional theory

O-07: Exploring the effect of Jahn-Teller distortion on Electrocatalytic activity of MoO_3

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Abstract:

Heterogeneous catalytic activity of a catalyst is purely dependent on the crystal plane exposed in the active surface and vacancies created to tune the acid-base behaviour[1–5]. Nucleation and directional growth of a crystal plane is mainly dependent on distortion and strain within the lattice due to which vacancies are created in the crystal[6]. In the present work we mainly focus on the synthesis, characterization and electrocatalytic application of molybdenum trioxide. Microwave-assisted hydrothermal synthesis of $MoO_3$was made using ammonium molybdate as a molybdenum precursor in acidic medium. The synthesized materials are characterized by powder XRD, FT-IR, DRS, SEM, BET to understand the crystal structure, composition, band gaps, morphology and microstructural properties of as prepared compounds. The changes in band gap are in coherence with the crystallite size of the compound prepared. It is observed that the concentration of precursor salt used, has shown a significant change in the morphology. Through rietveld refinement analysis we are able to draw the bonding parameters and lattice structures. The electrocatalytic activity of prepared compounds has been checked for Direct Methanol oxidation reaction and it shows a significant change in the activity with change in crystal facets.

Keywords: Molybdenum oxide, electrocatalyst, rietveld refinement, methanol oxidation

O-08: MoS_2 and Janus (MoSSe) based van der Waals Heterostructures as an emerging direct Z-scheme photocatalysts

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Abstract:

MoS_2 monolayer, a prototypical transition metal dichalcogenide (TMD), with high carrier mobility and apt optical properties have often been used in photocatalysis. Janus (MoSSe) too follows the same. However, the usage of these monolayers is limited by the carrier (e^--h^+) recombination, making it imperative to examine their bilayer van der Waals heterostructure (vdW HTS), where the spatial separation of e^--h^+ on two layers reduce recombination. The design of bilayer vdW HTSs here, consists of TMDs (HfS_2, ZrS_2, TiS_2, WS_2) and transition metal oxides (TMOs) (HfO_2, T-SnO_2, T-PtO_2). The present work displays curiosity in their Z-scheme photocatalytic capability, where faster interlayer e^--h^+ recombination as compared to that of intralayer, is required for efficient spatial charge separation and hence, redox reactions. We have performed first-principles based calculations under the framework of (hybrid) density functional theory (DFT) and many-body perturbation theory (GW approximation), to obtain the band edge levels and optical spectra, respectively. The comparative study of vdW HTSs and the constituent monolayers, have been undertaken by analyzing their band edge alignment, electrostatic potential, work function, charge transfer and e^--h^+ recombination. As per the systematic analysis of aforementioned parameters along with promising optical response the inferred vdW HTSs are MoSSe/HfS_2, MoSSe/TiS_2, MoS_2/T-SnO_2 and MoSSe/ZrS_2. Finally, on comparing their hydrogen evolution reaction (HER) capability with that of MoS_2 and MoSSe monolayers, we report them as probable Z-scheme photocatalysts.

Keywords: Z-scheme photocatalysts; Janus; van der Waals heterostructure

O-09: Role of Fe doping in NiOOH monolayer for water oxidation catalysis - A first-principles study

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Abstract:

A key obstacle to the success of electrochemical water splitting is the oxygen evolution reaction (OER), a kinetically inefficient but crucial half-reaction.1 OER is a significant contributor to the overpotential as it involves the exchange of four protons and electrons as well as an O-O bond formation, necessitating the use of catalysts. Ni based hydroxides and oxyhydroxides are recognized as highly active electrocatalysts for water oxidation in basic medium.2 The OER activity of pristine NiOOH is enhanced by doping with Fe.3 However, the precise role of Fe is still being debated. Here, we use the first-principles DFT+U approach to study three different types of active sites: one on pristine and the other two on Fe-doped NiOOH monolayers to account for the direct and indirect roles of Fe. To compare the activity of the active sites, we consider two Mars-Van-Krevelen mechanisms of OER based on the source of O-O bond formation. Our results show that the mechanism involving the coupling of lattice oxygen (LOC) is generally more favorable than water nucleophilic attack (WNA) on lattice oxygen. On doping with Fe, the overpotential of NiOOH is reduced by 0.33 V in excellent agreement with experimental findings. Introducing Fe at active sites results in different potential determining steps (PDS) in the two mechanisms, whereas Ni sites in pristine and Fe-doped NiOOH have the same PDS regardless of the mechanism. The Fe sites not only have the lowest overpotential but also decrease the overpotential for Ni sites.4

Keywords: Metal oxyhydroxide; oxygen evolution reaction; lattice-oxygen coupling mechanism, density functional theory

References:

1. Anantharaj, S. et al. *ACS Catalysis* **2016**, 6, 8069–8097
2. Fidelsky, V. et al. Theor. Chem. Acc. **2016**, 135, 162
3. Martirez, J. M. P.; Carter. E. A *J. Am. Chem. Soc.* **2019**, 141, 693–705
4. Kumar, M. et al. ChemRxiv **2021**, DOI: 10.33774/chemrxiv-2021-kthjg

O-10: Fabrication of Tin (Sn) based 2D materials & its device applications

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Abstract:

In the light of recent advances in 2D material family, Layered metal dichalcogenides (LMDCs) with their notable properties and next generation optoelectronic & photonic applications amplified the interest & attention. SnS_2 a tin (Sn) based 2D material isoelectronic with graphene belongs to a class of LMDCs. Unlike other LMDs like WS_2 & MoS_2, both the bulk & single layer SnS_2 possess indirect band gap. It is a n-type semiconducting material with an indirect band-gap of 2.2 - 2.35 eV. SnS_2 with hexagonal crystal structure has unique characteristics including high carrier mobility, fast photo response, good photo catalytical activities & high optical absorption. Earth abundancy, nontoxicity & environmentally friendly nature of SnS_2 made it suitable for some sustainable electronic applications.

Here our main focus is to fabricate SnS_2 using various deposition techniques like PVD, CVD and device fabrication with hetero stacking of other 2D materials. Also, we study the temperature dependent polytypism of SnS_2 with various substrates. The physical and chemical properties of the formed SnS_2 layers were studied with multiple characterization techniques including X-ray diffraction (XRD), Glancing incidence X-ray diffraction GIXRD, Transmission electron microscopy (TEM), Scanning electron microscopy (SEM), Atomic force microscopy (AFM), X-Ray photoelectron spectroscopy (XPS), Photoluminescence (PL) & Raman spectroscopy are used to characterize film structure, orientation, morphology, composition, optical bandgap of SnS_2 film. Our non-conventional synthesis methods & experimental findings may lead to future directions & opportunities for the optoelectronic & energy storage device applications of 2D materials family.

Keywords: LMDCs; optoelectronics; photonic; hetero stacking; device applications

O-11: CO_2 to methanol reduction on S vacancy rich MoS_2 monolayers: 2H v/s 1T phase

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Abstract:

CO_2 is a potential feed-stock for renewable source of energy which can be used to produce carbon-neutral fuels and chemicals. However activation of CO_2 itself is very challenging due to its high bond dissociation energy. Another challenge among researchers include over-reduction of CO_2 to less desirous products like methane. However, these challenges can be overcome using suitable catalytic system. Recently it was reported that 2H MoS_2 nanosheets containing in plane S vacancies can selectively reduce CO_2 to methanol at low temperature [1]. According to other studies, S vacancies are also responsible for 2H to 1T phase transition [2]. Taking motivation from these studies, we are considering coexistence of both the phases within same catalyst, competing each other to provide CO_2 activation site. Using Density Functional Theory, we are trying to investigate activity of S vacancy rich 2H and 1T mono-layers towards CO_2 reduction to value added products. In this work, we have studied CO_2 reduction on S vacancies at varying concentration and distributions on both 2H and 1T phases. Though the strength of CO_2 interaction with S vacancies is similar on both the phases, adsorption in 1T induces structural transition to 1T' phase. Computational Hydrogen Electrode (CHE) model have been implemented in order to understand reaction pathway and selectivity of one product over other. Formate formation was more favorable on S vacancies compared to pristine mono-layers in both the phases. Among different mono-layers studied, S vacancies in 1T' phase show better response towards CO_2 reduction to formic acid and methanol via formate pathway.

Keywords: CO_2 reduction, MoS_2 mono-layers, S vacancy, methanol, formic acid

O-12: Design and characterization of some organic diradicaloids

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Abstract:

Organic diradicaloids, which have various electronic applications like singlet fission, molecular electronics, non-linear optics, NIR photodetectors etc are designed with Donor -π-donor and Acceptor -π-acceptor molecular skeleton. Beyond multireference methods, we calculated the diradical character (y_0) of these molecules using DFT Hybrid functional, to reduce computational cost. The static electron correlation, which is a measure of diradical character, is calculated by FOD analysis.

Keywords: Diradicaloid; Diradical character(y_0); FOD (fractional occupation weighted density); SEC (static electron correlation)

O-13: First-principles study of Skutterudite/Nb interface at high temperatures for thermoelectric applications

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Abstract:

Thermoelectric devices convert heat energy into electrical energy and are of great importance in the search for clean and sustainable energy. Most studies in this area focus on developing more efficient thermoelectric materials (TM). The performance of a thermoelectric device also depends on the quality and stability of the interface between the thermoelectric component and the electrode material, particularly at the high-temperature end of the device. However, this aspect is not well studied.

Filled skutterudites are promising TM to be used at high temperatures (usually > 800 K). In this work, using a combination of density functional theory-based calculations and Born Oppenheimer molecular dynamics (BOMD) simulations, we have studied the interface between (001) surfaces of Ba half- filled CoSb3 Skutterudite and (110) Niobium surface, the latter being used as an electrode.

For Ba0.5Co4Sb12, depending on the Ba and Sb chemical potential either the Ba or Sb terminations were most stable. Upon the formation of the interface, we observe that the skutterudite lattice parameters are stretched along the x-y plane. The interface with both Sb and Co at the interface is found to have the lowest binding energy (BE) of -1.97 J/m2 and there is an accumulation of charge density at that interface. The interfaces with Ba at or close them have relatively higher BE.

The above interface was determined using DFT calculations that are usually done at 0K. Presently we are performing finite temperature BOMD simulations to study the effect of the temperature on the structure of the interface.

Keywords: Thermoelectric; Skutterudites; electrode interface; Density Functional Theory; Born Oppenheimer Molecular Dynamics

O-14: Materials Genome Initiative (MGI)-Accelerating Materials Innovation

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Abstract:

Looking to the fast technological development in overall modern information technology industry, the development of advanced materials will fuel many of the emerging industries that will address challenges in energy, cyber security, healthcare, and other areas of manufacturing. Yet the time it takes to move a newly discovered advanced material from the laboratory to the land or industries place remains far too long. Speeding this process could significantly improve global competitiveness and ensure that the world remains at the forefront of the advanced materials marketplace. This Materials Genome initiative for Global Competitiveness aims to minimize development time by providing the suitable infrastructure and training that researcher need to discover, develop, manufacture, and apply advanced materials in a more economical way.

A genome is a set of information encoded in the language of DNA that serves as a blueprint for an organism’s growth and development. The Materials Genome Initiative (MGI) is a new, multi-stakeholder effort to develop an infrastructure to accelerate advanced materials discovery and deployment. This new focused initiative will better leverage existing investments through the use of computational capabilities, data management, and an integrated approach to materials science and engineering. This paper describes a vision of how the development of advanced materials can be accelerated through advances in computational techniques, more effective use of standards, and enhanced data management.

Keywords: Material Genome, data management, computational techniques

O-15: Evaluation of various deep learning approaches for mechanical property prediction in austenitic stainless steels

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Abstract:

Austenitic stainless steel (ASS) has found their application in various fields including pressure vessels, heat exchanger, aerospace, marine, defense, household appliances, etc. ASS has been used in as-cast form and processed form. The current research has used ASS in quenched condition. Dataset consists of chemical composition, quenching medium (air and water), heating temperature, and time duration of heating as controllable input variables and Ultimate Tensile Strength (UTS) and Yield Strength (YS) as responses. Artificial Neural Networks (ANNs) have been employed to predict the responses as a function of input variables. With the constant 150 epochs, various optimizers and activation functions have been used for the analysis. Mean Absolute Error (MAE) has been taken as a measure of performance. Along with MAE, time required for training has also been recorded. An optimum combination of optimizer and activation function considering MAE and training time has been suggested as an outcome of the research.

Keywords: Austenitic stainless steel, Artificial Neural Networks, Mean Absolute Error

O-16: DFT Study on the Physical Properties of LaCoTiIn Equiatomic Quaternary Heusler Alloy for Spintronics and Thermoelectrics

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Abstract:

We have evaluated the structural, mechanical, thermal, electronic, magnetic, and transport properties of LaCoTiIn equiatomic quaternary Heusler alloy using density functional theory. The Generalized Gradient Approximation (GGA) and GGA+U schemes have been used as exchange-correlation functional for the above calculations. From the ground state calculation, LaCoTiIn EQHA with a Type-III structure in the ferromagnetic (FM) state is found to be stable. The electronic structure of LaCoTiIn EQHA depicts half-metallic behavior which has metallic overlap in the spin up (↑) channel and a semiconductor band gap in the other channel. The spin–orbit coupling of LaCoTiIn has a great influence on the band gap of the material. The computed band gap values for the spin down (↓) channel are 0.480 eV and 0.606 eV by using the GGA and GGA+U schemes. The total spin magnetic moment is 1 μB, according to the Slater–Pauling rule, $M_{\text{Tot}} = (Z_{\text{Tot}} - 18)\ \mu B$. The small band gap in the minority spin channel enhances its thermoelectric characteristics. The stable half-metallicity, high Curie temperature, high electrical conductivity, small thermal conductivity, and good figure of merit all point to this material as a good choice for spintronic and thermoelectric devices.

Keywords: Heusler Alloys; Density Functional Theory; Half-metal, Spintronics; Thermoelectrics

O-17: Exploring the Efficiency of Carbon Nanostructures for Hydrogen Storage and Oxygen Reduction Reaction

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Abstract:

First-principles density functional theory has been employed to explore new carbon allotropes such as, carbon nanohorn and T6-carbon for the purpose of hydrogen storage and oxygen reduction reaction (ORR) respectively. In this presentation, I will explain how the presence of curvature can be exploited as a tuning parameter to activate the hydrogen storage capability of single-walled carbon nanohorns (SWCNHs). The binding strength of ad-atoms on SWCNHs of different curvature is correlated with the π electron occupancy of the corresponding carbon ring. Higher π electron occupancy causes significantly high binding energy of the metal ad-atoms (M), thereby indicating high stability of those M-C bonds. After full hydrogenation, Li-doped SWCNHs are found to contain a maximum of 7.5 wt. % of hydrogen. Overall, our results indicate that Li-doped SWCNHs with intra-curvature values higher than 11^{o}, is a potential candidate for hydrogen storage. I will also explain the electro-catalytic activity of a new carbon allotrope i.e. T6[100] surface containing both *sp*3 (C1) and *sp*2 (C2) hybridized carbon atoms for efficient ORR. As estimated from free energy profile, the overpotential is much lower when C1 is considered as the active site and the final step i.e. desorption of final OH- ion is found to be the potential determining step. Thus, the presence of both *sp*2 (maintains the high metallicity needed to reduce ohmic loss) and *sp*3 (helps in capturing the upcoming molecules) hybridized carbon atoms in T6[100] surface helps it to act as a potential candidate for ORR.

Keywords: carbon nanohorn; curvature; π electron occupancy; T6-carbon; Overpotential

O-18: First-principles insight on the atomic arrangement of wurtzite (B, Al, In)$_{0.125}$Ga$_{0.875}$N and its implications in crystal stability.

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Abstract:

Some fluctuations in composition are commonly observed in epitaxial-grown III-V multinary alloys. These fluctuations are attributed to compositional pulling effects and an insight on their atomistic origin is necessary to improve current epitaxial growth techniques. In addition, the crystallinity of III-V multinary alloys varies widely depending on the constituent atoms. Using first principles calculations, we then investigated different geometric configurations of gallium nitride (GaN)-based ternary alloy, $X_{0.125}Ga_{0.875}N$ where X is the minority atom which is either boron (B), aluminum (Al), or indium (In). The minority atoms are presented as two atoms in the simulation cell, and the energetics of five geometric configurations are analyzed to estimate the most stable configuration. For the $B_{0.125}Ga_{0.875}N$ alloy, the most stable configuration is the one where the minority atoms occupy gallium (Ga) sites in a collinear orientation along the c-axis. On the contrary, the configurations along the in-plane direction result in a higher energy state. $In_{0.125}Ga_{0.875}N$ and $Al_{0.125}Ga_{0.875}N$ also show the same trend with a small relative energy difference. These preferential sites of minority atoms are consistent with composition pulling effects in wurtzite nitride phases. Moreover, the degree of crystallinity for wurtzite nitride alloys can be well described by the order of calculated relative energy.[1]

Keywords: crystal structure; semiconductor; ternary alloys

O-19: Effect of pore structures of carbon support on the electrode reaction activity of the catalyst layer in polymer electrolyte fuel cells: Reactive molecular dynamics simulation

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Abstract:

For large output of polymer electrolyte fuel cells (PEFCs), the electrode reaction activity of the catalyst layer (CL) consisting of carbon supports, Pt nanoparticles, Nafion chains, and water should be improved. According to the previous studies, when Ketjen Black (KB) with meso pores is used as the carbon support, electrode reaction activity of the Pt nanoparticles is higher compared with carbon black supports without pores and the electrode reaction activity depends on the pore structures of the KB support. Therefore, elucidating the effect of the pore structure of the KB support on the electrode reaction activity of the CL contributes to the improvement of the electrode reaction activity and output of PEFC. In this study, to clarify the effect of pore size on the electrode reaction activity of Pt nanoparticles in the CL, we investigated the CL structure with a different pore size of the KB support by reactive molecular dynamics method. To discuss the electrochemical activity of the Pt nanoparticles, we evaluated the connectivity of the Nafion chains to H2O molecules absorbed on the Pt nanoparticles on the exterior and in the interior of the pores because the Nafion chains conduct the protons to the H2O molecules on the Pt nanoparticles. As the pore size increases, more Nafion chains have penetrated the interior of the pore and contact with H2O molecules on the Pt nanoparticles. This suggests that the large pore size promotes the formation of a proton-conducting path composed of the Nafion chains, H2O, and Pt nanoparticles, leading to high electrode reaction activity.

Keywords: Reactive Molecular Dynamics; Polymer Electrolyte Fuel Cell; Catalyst Layer; Ketjen Black; Reaction Activity

O-20: Reactive molecular dynamics simulation of corrosion wear of DLC/Fe sliding interface in the presence of water and oxygen in automobile engines

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Abstract:

To improve the fuel efficiency of automobiles, an exhaust gas recirculation system in which a portion of an engine's exhaust gas is circulated to an engine cylinder is used. However, impurities in the exhaust gas have been noted to cause corrosive wear at the sliding interface between the diamond-like carbon (DLC) coated piston and the steel cylinder. Previous studies have shown that NO*x* in the exhaust gas dissolves into flocculated water, as a result, nitric acid which causes corrosive wear is generated. To improve the durability of automobile engines, it is necessary to clarify the relationship between corrosive wear and the chemical reactions of various molecules such as water, oxygen, nitric acid, and oil at the sliding interface. However, it is difficult to investigate the chemical reaction process at the sliding interface from experiments. In this study, we used reactive molecular dynamics simulation to analyze the chemical reactions at the sliding interface of DLC/Fe in aqueous and oxygen-containing aqueous environments. We found that when the Fe and DLC substrates came into contact with each other, the Fe atoms were scraped off and adhered to the DLC surface with a formation of Fe-C bonds. Meanwhile, Fe-O-Fe structures and Fe-O-H structures were formed on the Fe surface by chemical reactions with water and oxygen. We also found that the dissolved oxygen promoted the formation of Fe-O-Fe structures and suppressed the formation of Fe-C bonds. We concluded that the enhancement of the Fe-O-Fe structure formation by dissolved oxygen is effective in reducing Fe-C bonds that induce the adhesion between Fe and DLC surfaces.

Keywords: Friction; Corrosion; Reactive molecular dynamics; Diamond-like carbon; Iron

Poster Presentation

P-01: Lowering the C-H Bond Activation Barrier of Methane Using SAC@Cu(111): A Periodic DFT Investigation

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Abstract:

Methane has long captured the world's spotlight for being the simplest and yet one of the most notorious hydro carbon. Exploring its potential to be converted into value added products has raised a compelling interest [1-4]. In the present work, we have studied the efficiency of Single-Atom Catalysts (SACs) for methane activation employing Density Functional Theory (DFT). The Climbing Image Nudged Elastic Bond (CI-NEB) method is used in tandem with the Improved Dimer (ID) method to determine the minimum energy pathway for the first C-H bond dissociation of methane. Our study reported that the transition-metal doped Cu(111) surfaces enhance adsorption, activate C-H bond, and reduce activation barrier for first C-H bond cleavage of methane. The results suggest Ru/Co/Rh doped Cu(111) as promising candidates for methane activation with minimal activation barrier and less endothermic reaction. For these SACs, the calculated activation barriers for first C-H bond cleavage are 0.17 eV, 0.24 eV, and 0.26 eV respectively, which is substantially lower than 1.13 eV, the activation barrier for Cu (111).

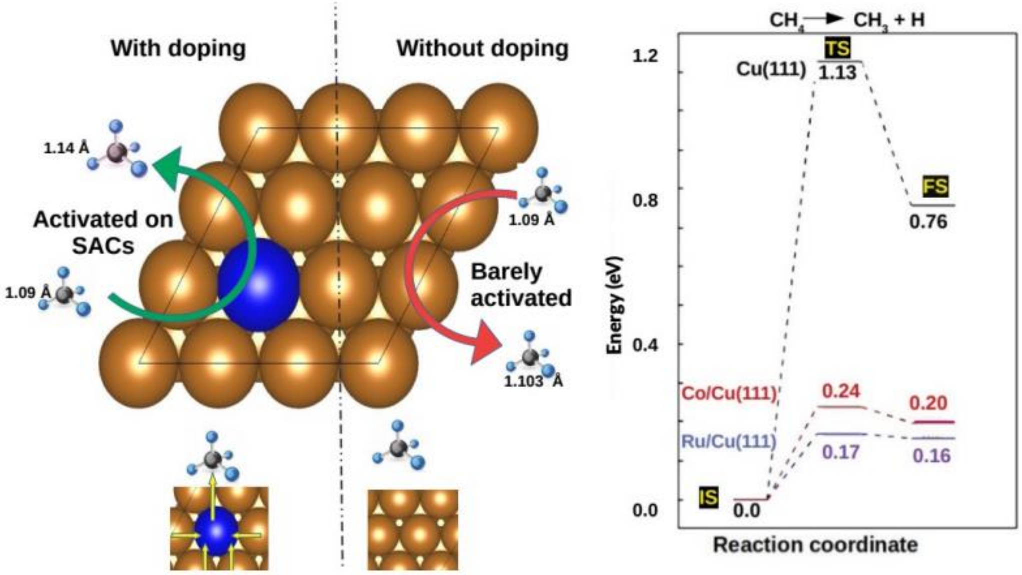

Figure 1 Pure Cu(111) and TM/Cu(111) SAC surfaces and reaction path for first C-H bond dissociation on Pure Cu(111) and TM/Cu(111) surfaces.

P-02: Looking beyond adsorption energies to understand interactions at surface using machine learning.

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Abstract:

Investigating the activation of molecules on metal surfaces is a starting point for understanding catalysis. Identifying factors that influence interactions at the surface is still an active area of research. In this study, we present the importance of analyzing bondlength activation, while interpreting Density Functional Theory (DFT) results, as yet another crucial indicator for catalytic activity. We studied the adsorption of small molecules, such as O_2, N_2, CO, and CO_2, on seven face-centered cubic (fcc) transition metal surfaces (M = Ag, Au, Cu, Ir, Rh, Pt, and Pd) and their commonly studied facets (100, 110, and 111). Through our DFT investigations, we highlight the absence of linear correlation between adsorption energies (E_{ads}) and bond-length activation (BL_{act}). The two parameters are expected to be correlated for any interaction between an adsorbate and a catalyst surface. But a careful analysis proves the lack of linear correlation between the two. Our study indicates the importance of evaluating both to develop a better understanding of adsorption at surfaces. We also developed a Machine Learning (ML) model trained on simple periodic table properties to predict both, E_{ads} and BL_{act} . Our ML model gives an accuracy of Mean Absolute Error (MAE) $\sim$ 0.2 eV for E_{ads} predictions and 0.02 Å for Bl_{act} predictions. The systematic study of the ML features that affect E_{ads} and BL_{act} further reinforces the importance of looking beyond adsorption energies to get a complete picture of surface interactions with DFT.

Keywords: Density functional theory, Machine learning, Bond-length activation, Activation trends

P-03: Interaction of methanol with metal oxide: from computation to experiments.

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Abstract:

Metal oxides exhibits better catalytic activity than pure metals due to the presence of acidic and basic sites on their surface. Metal oxides are essential catalyst in synthesis of various value-added chemicals via oxidation, dehydrogenation, acid-base reactions etc. Methanol, being a prominent hydrogen source, has a potential to replace the existing fuels. However, conversion of methanol to any value added product, requires breaking of its O-H and/or C-H bond. The Edisonian approach of catalyst improvement or discovery demands humongous lab scale experiments, which are costly and time consuming. Use of computation offers not only flexibility but also accelerate the search by providing a platform to carry out virtual experiments. Since the computation is based on solid foundations of Density Functional Theory (DFT), the underlying electronic structure provides atomistic level insights about functioning of a catalyst. Here, I would like to discuss about employment of DFT to unravel interaction of methanol with metal oxide and mixed metal oxide. Our DFT investigations show spontaneous dissociation of O-H bond of methanol on both the surfaces. Different facets of a catalyst exhibit different activity towards methanol. With the help of electronic structure, we provide rationale as to why these surfaces works better for methanol dissociation. The metal oxide surface presents spontaneous dehydrogenation of methanol to formaldehyde. To validate the DFT results, we designed lab scale experiment on the metal oxide, which also indicates synthesis of formaldehyde at ambient conditions.

Keywords: Metal Oxides, Methanol, formaldehyde, DFT

P-04: Visible Light Driven Nanoarchitectonics CZTS Thin film for Photocatalytic Application

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Abstract:

It is estimated that 70% of earth's surface is covered by water, out of which only 4% is clean or drinkable. In Present days water pollution has turned out as a major problem worldwide. Most of the pharmaceutical, chemical and textile industries discharge the effluent directly to fresh water such as lake and river. This effluent contains dye which is extremely hazardous to health as well as to the local ecology. Therefore, the degradation of the dyes from the effluent before it discharges to water body, has become a serious challenge. Dyes could be degraded through the process of photocatalysis in which the dye is dissociated to non-toxic components in the presence of light with the help of a catalyst. In this work we have investigated the photocatalytic property of visible light active CZTS thin film as an alternative to the usual metal oxide systems, which utilizes UV light. CZTS thin film was deposited in a single step using an ultrasonic spray pyrolysis instrument. XRD and Raman spectroscopy studies revealed that CZTS thin films possess kesterite structure. These thin films were used to degrade the 0.01mM methylene blue dye (as a test dye) under the visible light environment. 90% of the dye was degraded in a duration of 2h. Repeatability test was performed for 5 times to check the adhesion properties and stability of the films and it showed good repeatability. CZTS thin films shows that it can degrade the dyes better in base medium than acidic medium. Degradation rate for MB is found to be in 0.02086 min^{-1}.

P-05: Theoretical investigation of the Pt/water interface using QM/MM based path integral molecular dynamics.

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Abstract:

Electrode-electrolyte interfaces have been of immense interest in the field of energy storage and conversion. In particular, the hydrogen evolution reaction (HER) at the Pt/water interface is one of the most important reactions for hydrogen storage. The description of the water-water and metal-water interaction at the interface is crucial as it influences the work function of the metal thereby affecting its catalytic activity for hydrogen evolution. The hydrogen-bonding is important in water and since the hydrogen atoms are light, it would be interesting to understand how the nuclear quantum effects (NQE) influence the interface properties. Studying this interface using experimental and theoretical tools is challenging. Therefore, in this work, we show that using QM/MM based path integral molecular dynamics (PIMD) simulations, NQE at the Pt(111)-water interface could be studied at a lesser computational cost while retaining the information available from the expensive *ab initio* PIMD simulations. We observed that the interface water forms a bilayer namely the wetting and non-wetting layer. The wetting layer consists of dissociated OH- ions directly binding on top of Pt through the oxygen atom whereas the non-wetting layer is populated by the dissociated hydrogen atoms from the wetting layer to have positive ions (H3O+ and zundel ions). The non-wetting layer forms hydrogen bonds with the second water layer beyond which properties of bulk water are restored. We also observed there is a net transfer of electronic charge from the water bilayer towards the Pt atoms. The formation of ionic species along with the charge transfer induce local dipole moments which influence the work function of the Pt metal.

P-06: Effect of spin-orbit coupling and anti-site disorder on thermoelectric performance of Half Heusler alloy LaPtSb

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Abstract:

Thermoelectric effect is a green way of converting waste heat into electrical energy. In this work, using density functional theory (DFT) based calculations, we are investigating the effect of spin-orbit coupling and antisite disorder on the electronic and transport properties of a theoretically predicted Half Heusler alloy, namely LaPtSb. Here antisite disorder arises by exchanging the positions of Pt and Sb atoms. While the pristine compound is a semiconductor with a band gap of 0.62 eV (using hybrid functional), the one with 100% disorder is a semimetal with the valence and conduction band touching each other at the Γ-point of the Brillouin zone. Upon incorporating the spin-orbit coupling (SOC) interactions, for the pristine case, the band structure reduces to 0.45 eV. Interestingly, for the disordered one SOC results in slight opening up of the band-gap (0.08 eV). Further analysis shows that for both these cases one observe Rashba splitting of the bands. While in pristine LaPtSb the Rashba splitting energy is 1.15 meV and the offset in k-space is 0.010 A-1, for the 100% disorder these are 0.152 eV and 0.089 A-1. For the intermediate concentrations of disorder, we observe that the material becomes metallic (without SOC and hybrid functionals). Presently more studies on the effect of SOC and hybrid functionals on these disordered systems are going on following which we will be studying the effect of these changes in the band structure on the transport properties. Additionally, we are also studying the effect of strain onthese systems.

P-07: Thermoelectric properties of full Heusler alloy Fe2VIn1- xGax

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Abstract:

Thermoelectric materials provide the direct conversion of heat into electrical energy. In recent years, Heusler alloys have attracted significant attention because of their large power factor however, the efficiency of these materials is still very low due to high lattice thermal conductivity. In this study, We report the structural, electronic, and thermoelectric properties of a full Heusler alloy Fe2VIn1-xGax where (x=0,0.25,0.5,0.75,1.0). Fe2VIn and Fe2VGa crystallize in a face-centered cubic (fcc) structure where Fe is in a tetrahedral environment with V and Ga/In. Substitution of Ga in Fe2VIn varies the lattice parameter linearly following Vigard's law. The electronic properties of the alloys Fe2VIn1-xGax predict these to be metallic in nature. The substitution of Ga into Fe2VIn distorts the local tetrahedral environment and leads to significant changes in the band structure and density of states near the Fermi energy. These changes significantly affect the transport properties of the system. In particular, the Seebeck coefficient of the Fe2VIn and Fe2VGa are 35 µV/K and 32 µV/K upon hole doping at 300 K. The substitution of Ga leads to further enhancement in the Seebeck coefficient, and the maximum Seebeck coefficient was found to be 65 µV/K for Fe2VGa0.5In0.5 at 300 K. We notice a significant improvement in electrical and electronic thermal conductivity of the alloy Fe2VIn1-xGax because of the decreased scattering rate of carriers and suitable band structure modification. We estimate the lattice thermal conductivity of the alloys using Cahill's model and found that lattice thermal conductivity has increased due to increase in the phonon group velocities of the alloys. These enhancements in transport properties of the alloy improve the thermoelectric figure of merit (ZT) to be 0.14 for hole doping at 300 K which is 0.05 for Fe2VIn at 300 K.

P-08: Descriptors and graphical construction for in silico design of efficient and selective single atom catalysts for eNRR

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Abstract:

The electrochemical nitrogen reduction reaction (eNRR) offers the possibility of ammonia synthesis under mild conditions; however, it suffers from low yields, a competing hydrogen evolution reaction pathway, and hydrogen poisoning. We present a systematic approach toward screening single atom catalysts (SACs) for eNRR, by focusing on key parameters computed from density functional theory, and relationships between them. We illustrate this by application to 66 model catalysts of the types, TM-Pc, TM-N_XC_Y, and TM-N_3, where TM is a 3d transition metal or Molybdenum. We identified the best SACs as Sc-Pc, Cr-N_4, Mn-Pc, and Fe-N_2C_2; these show eNRR selectivity over HER and no hydrogen poisoning. The catalysts are identified through multi-parameter optimization which includes the condition of hydrogen poisoning. We proposed the new electronic descriptor O_{val}, the valance electron occupancy of the metal center, that exhibits a volcano-type relationship with eNRR overpotential. Our multi-parameter optimization approach can be mapped onto a simple graphical construction to find the best catalyst for eNRR over HER and hydrogen poisoning.

Keywords: eNRR, Adsorption, Electrocatalyst, DFT, HER, Descriptor

P-09: Nitrogen and Boron Co-ordinated ideal dual site catalyst for CO oxidation

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Abstract:

Single Atom Catalysts (SACs) are extensively used in different areas of research due to their high catalytic activity and selectivity. SACs supported with carbon-based surfaces are widely used in characterization and synthesis due to its large specific surface area and electrical conductivity with unique chemical properties. Nitrogen affects the catalytic activity of surface towards CO oxidation. Nitrogen doping in double vacancy graphene increases the binding energy of transition metal atom on the substrate, enabling the formation of stable single atom catalysts. Binding energies of metal atom on the surfaces decreases the binding of oxygen molecule on metal atom. Results revealed that the additional incorporation of boron along with nitrogen into metal SACs leads to provide more active sites on the surface to impart a synergetic effect for boosting catalytic performance.

In this work we have systematically investigated the adsorption of O2 and CO molecule on 3d (Ti, V, Cr, Mn, Fe, Co, Ni, Cu) transition metal single atoms anchored on N4, N3, N2 and N2(op)-doped graphene using the DFT calculations. As, the transition metals binds more strongly to the vacancy, it binds oxygen less strongly i.e. on such systems possibility of CO poisoning will be more. Further, the CO oxidation mechanism catalyzed by the metal-boron dual atom site was then investigated. We found that the variation in adsorption energy of O2 molecule for each metal is traceable to variations in the electronic structure. The contribution of the five d orbitals to chemisorption of molecule is different. Values of d-band are then calculated individually making role of t_{2g} (dxz + dyz + dxy) and e_g (dx^2-y^2 + dz^2) more accurate in general. While examination of the relationship between adsorption energy of molecule and d-band of individual orbitals, we find that the adsorption energies can be fit as a linear function of e_g. This result demonstrates that focusing on the metal orbitals involved in bonding simplifies the observed adsorption behavior.

P-10: Fabrication of α-MoO_3 layers and conversation to MoS_2.

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Abstract:

We referred in this abstract with two types of synthesis methods on nanostructures of molybdenum trioxides. Transition metal oxides (TMOs) such as MoO_3 have been researched for so many years due to their remarkable applications in electronics, gas sensors, LEDs, photo, electrochromic materials, and the rest. MoO_3 is classified into two types. They are α- MoO_3 in orthorhombic and β- MoO_3 in monoclinic shapes. β- MoO_3 is the metastable phase that is transformed into the α-phase by heating above 673K. We used Physical vapour deposition to grow molybdenum thin films on different substrates. Deposited Mo thin films in PVD used as a source in chemical vapour depositions and Hot plate to grow multilayers of MoO_3 on graphene/SiO_2 as a substrate with temperature variations. Hot plate and CVD are done in ambient conditions but PVD is done in high vacuum regions. Thermal evaporation techniques give a single crystal form.

The characterization of MoO_3 thin films were studied in X-ray diffraction (XRD), Glancing incidence X-ray diffraction (GIXRD), Scanning electron microscopy (SEM), Raman spectroscopy, and dielectric measurements. We observed the information of crystal structure, impedance, orientation, surface morphology and optical images of MoO_3. To know the light transmittance and emission spectra of MoO_3 thin film, we used UV-Vis spectroscopy and Photoluminescence (PL) spectra.

Keywords: Transition metal oxides (TMOs), Molybdenum trioxide (MoO_3), PVD, CVD.

P-11: Corrosion prevention through High entropy alloys (HEAs) coating

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Abstract:

The global cost of corrosion is estimated to be US $2.5 trillion, which is equivalent to 3.4% of the global GDP. India loses around Rs 1.52 lakh crore annually**, w**hich is around 5-7 % of its Gross Domestic Product (GDP) every year due to corrosion in various sectors including infrastructure, utility services, production & manufacturing, defence & power plant. Therefore, the preparation of highly corrosion - resistant material is requirement of the day. By making a new composition with high entropy alloys (HEAs) that possesses a unique microstructure that is made of solid solutions with random arrangements of multiple elements. Sometimes, as an effective means for the economic justification, surface coatings have drawn extensive attention in the field of material corrosion. This paper describes the methodology, different elements effects for producing excellent corrosion resistance of (HEAs) coatings.

Keywords: High entropy alloys (HEA), Corrosion, Corrosion Resistance Alloys (CRA), High entropy alloys (HEA) coatings

P-12: Origin of pure and C doped borophene stability and its activity for OER

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Abstract:

In borophene, vacancy is a major reason for stability. However, a detailed understanding relating to vacancy and electronic property remains unexplored. Using Density Functional Theory (DFT) the effect of vacancy and doping on stability, electronic and catalytic properties of borophene is addressed in this work. It is shown how vacancy increases σ-electrons and decreases π-electrons of the neighboring boron atoms with the magnitude decreasing from 4 to 6-coordinated atoms, thereby contributing to their stability. The role of single and dual carbon doping on σ- and π-occupancy is explored. In addition, we have shown that dual carbon doping on β12 borophene analogue reduces the overpotential for oxygen evolution reaction (OER). We observed that the charge deficient boron atom helps in the reduction of oxygen binding and can decrease the overpotential towards OER. Overall, this work would help in fundamental understanding towards borophene stability and aid in choosing the suitable dopant for catalytic applications considering the stability.

Keywords: DFT, borophene, electrocatalyst, OER

P-13: Investigating the origin of ferroelectricity and optical properties of molecular crystals CH_4N_2A (where, A = O, S, Se and Te) from first-principles calculations

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Abstract:

Molecular ferroelectric materials are promising to replace the well-known ferroelectric perovskite oxides due to their structural flexibility, tunability, and ease of processing. We started our investigation by considering experimentally synthesized thiourea (CH_4N_2S). The lattice parameters for thiourea are reportedly show a = 8.52 Å, b = 5.49 Å, and c = 7.54 Å with orthorhombic $Pmc2_1$ symmetry whereas based on DFT calculations after complete relaxation we obtained a = 8.37 Å, b = 5.44 Å, and c = 7.81 Å with same symmetry. The forbidden gap for CH_4N_2S is determined to be 3.5 eV. First-principles density functional theory calculations are used to explain the ferroelectric genesis of the molecular ferroelectric substances CH_4N_2A with A = O, S, Se, and Te. Herein, we report an improper ferroelectric origin of the working compounds through a group theoretical approach. We exploited that the ferroelectric materials CH_4N_2A are suitable for optical applications. Among them, we found CH_4N_2Te with bandgap energy $\sim$ 2.5 eV is even more interesting owing to large ferroelectric polarization, P = 10.92 $\mu C/cm^2$. We identified for the working materials, the origin of an increasing polarization behavior is associated with decreasing energy bandgap. In addition, we investigated the thermodynamic, and dynamic stability of each system, and are found to be stable.

Keywords: First-principles calculations; Molecular ferroelectrics; Band-engineering; Optical-applications

P-14: Exploring functional mode couplings in $(LaNiO_3)_1/(CaNiO_3)_1$ superlattice through first-principles calculations

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Abstract:

Multiferroics are fascinating for technological-oriented applications in various fields such as spintronics, structurally triggered insulator-to-metal transition, and so on. Perovskite nickelates in layers are potential candidates for spintronics, and insulator-to-metal transition due to partially filled t_{2g} or e_g crystal field splitting of the Ni-3d in layered $(La^{3+}Ni^{3+}(3d^7)O_3)_m/(Ca^{2+}Ni^{4+}(3d^6)O_3)_n$ superlattices where m, and n are both odd. We started our investigation based on first-principles study by constructing superlattices between rare earth nickelates ($RNiO_3$), and alkaline earth nickelates ($ANiO_3$). Interestingly, we found that our systems for any m, and n shows a ferromagnetic ground state. The ferromagnetic ground state with a trilinear mode coupling, $Q_{Tri} \sim Q_{Rot}Q_{Tilt}Q_{AFEA}$ (where Q_{Rot}, Q_{Tilt}, and Q_{AFEA} denote rotation and tilt of the NiO_6 octahedra, and antiferroelectric A-site displacements, respectively) can promote multiferroicity into the systems. Upon trilinear mode coupling, the systems not only show ferromagnetic ground state but also it offers us a half-metallic phase of the working superlattices. Hybridization of Ni-3d and O-2p states are found to responsible to obtain a half-metallic phase in $(LaNiO_3)_m/(CaNiO_3)_n$ superlattices. Further, we noticed that in ferromagnetic ground state, the systems give rise to a lower total magnetization because O-2p and N-3d are interacting antiferromagnetically. In addition, we found a few interesting phonon instabilities such as G-type charge disproportionation mode (Q_{GCD}) in analogy to the G-type anti-ferromagnetism, two-dimensional John-Teller distortions (Q_{JT}) mode which may open the energy gap and can promote a metal-to-insulator transition into the systems. Finally, we identified a multi-structural mode coupling, Q_M beyond the conventional Q_{Tri}, i.e., $Q_M \sim Q_{Tri}+ Q_{GCD}$ that leads the system to a polar $P2_1$ symmetry with even lowering the energy as compared to Q_{Tri}. We believe our findings will useful for future theory and experimental investigations.

Keywords: First–principles calculations, multiferroicity, ferromagnetism, nickelates, Half-metallicity

P-15: Design of Aluminium ion battery with Graphyne host: Lowest volume expansion, High stability and Low diffusion barriers

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Abstract:

Aluminum ion batteries (AIBs) are emerging as the promising alternatives to the Li-based battery technology. Commercialization of AIB requires limited volume expansion of the host cathode material after $AlCl_4$ intercalation, lower activation barrier, high theoretical specific capacity (TSC), cyclic durability and thermodynamical stability. Most of the carbon and non-carbon-based cathode hosts explored so far failed to address the issue of volume expansion and unclear about thermodynamical stability. Using first principles study, we explored the suitability of α and γ-Graphyne (GY) as cathode materials for AIB and observed that α-GY is the promising cathode host addressing each of the above concerns. Both α and γ-GYs provide large space to accommodate more number of $AlCl_4$ leading to a high TSC of 186 mAh/g and open circuit voltages of 2.18 and 2.22 V, respectively. The absence of bond dissociation for $AlCl_4$ and deformation of GY sheets at room temperature, as revealed from ab-initio molecular dynamics (AIMD) simulation, infer the stability of (α,γ-GY)+$AlCl_4$ systems. Intercalated α-GY shows a volume expansion of 186% which is lowest among the so far studied cathode materials. The negligible expansion energy (~ 0.003 eV/Å^2) ensures the reversibility and hence cyclic durability of α-GY. While the γ-GY shows a volume expansion of 249%, but still it is promising. The NEB based diffusion study estimates the activation barriers to be (0.26, 0.06 eV) for monolayer and (0.42, 0.16 eV) for bilayer of α,γ-GY, respectively. These values are either comparable or lower than that of the earlier reported cathode hosts.

Keywords: Aluminium ion battery, Graphynes, Diffusion energy barriers, Open circuit voltage, Volume expansion

P-16: Grain size dependence of thermal and electrical transport properties of nano-crystalline Sb_2Te_3 synthesized by mechanical alloying

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Abstract:

Antimony telluride (Sb_2Te_3) nanoparticles of different sizes were fabricated by mechanical alloying (MA) of elemental Sb and Te powers for different durations (3h, 5h and 10h). The powder nanostructures were pelletized, annealed in Ar atmosphere, and characterized by XRD, FESEM, EDX, TEM to explore the effect of milling time. The pelletized annealed samples were analyzed using a PPMS to study the effect of grain growth on their electrical and thermoelectric properties. The electrical resistivity increases with the grain size reduction, with increasing milling durations. The obtained positive values of the Seebeck coefficient indicate the p-type nature of the sample, which increase with milling time. The reduced thermal conductivity of the nanostructures with reduced grain size improves the thermoelectric figure of merit, ZT. The temperature-dependent Lorenz number ($L_{effective}$) is used to find the electronic contribution of total thermal conductivity, and the non-parabolic Kane model explains it. The much more dominant effect of thermal conductivity than electrical conductivity and Seebeck coefficient on the thermoelectric figure of merit causes a significant increase in ZT of the 10 h milled annealed sample compared to 3 h and 5 h milled samples.

Keywords: Mechanical alloying; Sb_2Te_3; Microstructure; Thermoelectric properties.

P-17: First principles identification of Novel Borophosphene/graphene heterostructure as a promising anode for future Li-ion battery

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Abstract:

As it is well known that graphite used as an anode for Li-ion battery (LIB), due to its low cost and conductive nature for ion and electrons. In recent years, after graphite, Si based or Si/C composite are also commercialized. Also, anode electrode required some properties viz (i) easy insertion, (ii) metallic nature, (iii) low volume expansion, (iv) high specific capacity and (v) moderate operating voltage. In our work, we have proposed Borophosphene and graphene based heterostructure. Since Borophophene is found metallic nature, with a dirac-cone, which helps Borophosphene/graphene heterostructure in conductivity. We have proposed possible diffusion path of Li-ion from one site to the other. We found that the diffusion energy required for these paths are in the range of 0.25 eV to 0.60 eV which is low as compared to graphite and Si/C composite. Also, the average open circuit voltage for this heterostructure is 0.0 - 1.0 volt. Since the interlayer distance is in the range of 3.45 Å, which helps for low volume expansion on Lithium insertion to the host structure. To know the other electronic properties, we have study charge density, band structure and to understand about the stability, we have studied the formation and volume expansion.

Keywords: DFT, Graphene, Borophosphene, heterostructure, LIB’s, Anode etc.

References: (1) First-principles identification of interface effect on Li storage capacity of C3N/graphene multilayer heterostructure, Deepak et. al., JCIS, 2021, 610, 80-88.

P-18: First Principles Study of Borophene As An Anode Material For Aluminum-ion Batteries

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Abstract:

Aluminum-ion batteries (AIBs) have emerged as a promising class of battery materials and have been intensively studied owing to their high theoretical capacity and reliable operational safety. In this work, the feasibility of using borophene as an anode material for AIBs was investigated through density functional theory (DFT). It was found that the adsorption of free Al atoms on the surface of borophene is energetically favourable. Upon the adsorption of Al atoms, we found that borophene retains its structural stability up to an Al concentration of 0.42. The metallic behaviour of both pristine and adsorbed borophene ensures the desirable electrical conductivity for batteries. Due to the trivalent nature of Al and the low molar mass of borophene, a high theoretical specific capacity of 3099 mAh/g is predicted, which is 8.3 times the value of commercial graphite anode. The buckled structure of borophene also allowed fast diffusion of Al along the direction of the furrow, having only a diffusion barrier of 27 meV. Our studies suggest that borophene is a potential anode material with high specific capacity and diffusivity for AIBs.

Keywords: borophene; aluminum-ion batteries; first principles calculations; density functional theory

P-19: Borophene as an energy storage device and catalyst for Hydrogen generation.

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Abstract:

The study and development of two-dimensional (2D) layered materials have gained interest among researchers worldwide. Two-dimensional (2D) boron sheets (borophenes) are promising materials for the next generation of electronic devices because of their metallic conductivity. Borophene, is a single layer of a boron atom, have been predicted theoretically and synthesized experimentally. The studies on Borophene have raised interest in different fields of Physics, Chemistry, and Material science, because it has many distinctive physical and chemical properties. Borophene finds its applications in diverse fields such as batteries, supercapacitor, sensors, hydrogen storage, and catalytic in hydrogen evolution. Here we aim to synthesize the Borophene by using CVD (Chemical Vapour deposition). The structural and texture properties are characterized by using Glancing angle incidence X-ray diffraction (GIXRD), Scanning electron microscopy (SEM), High-resolution transmission electron microscopy (HR TEM), Raman spectroscopy and Atomic force microscopy (AFM). The Current-Voltage measurements were done by using the Source measurement unit (SMU). The elemental compositions of borophene were analyzed by using X-Ray photoelectron spectroscopy (XPS). Our method paves the way for empirical investigations on borophene

Keywords: Borophene, supercapacitor; hydrogen storage.

P-20: First Principles identification of C2 Products by CO2 reduction of nanoparticle of Cu based alloy

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Abstract:

Converting carbon dioxide, a greenhouse gas, into fuels and chemicals not only contributes to reducing carbon dioxide emissions, but also provides energy security in a scenario of depletion of fossil resources (since non-renewable) and sharp fluctuations in oil prices (gradually depleting in near future). Unfortunately, activation of carbon dioxide to hydrocarbons like alcohol or ketone or aldehyde is itself a difficult task and finding the best catalyst with suitable composition, shape, size, high efficiency and cheap i.e. availability in long-term is a challenging problem. Copper is unique among metals in its ability to reduce carbon dioxide to such hydrocarbon products, especially methane, methanol, ethanol, ethylene and other organic products containing up to three carbon atoms.

This work describes our efforts to develop an appropriate catalyst, which has all the virtues mentioned above, for electrochemical CO2 reduction out of various copper-based nanoparticles having different composition, shape, size, and support therefore having different catalytic properties. In order to achieve the best catalysts, free energies of CO2 reduction intermediates in electrochemical reaction pathways on different facets of nanoparticles were calculated using density functional theory (DFT). We place greater emphasis on the Copper (111) facet because this surface exhibits a high selectivity for C2 products. After investigation on different copper surfaces by DFT calculations we found, On Cu55 (111), a proton is transferred to an adsorbate (such as the protonation of *CO to *COH) have small barriers on the order of 0.43 eV in C2 pathways. In contrast, the formation of *CHO from two adjacent *CO show barrier on the order of 0.7 eV in C1 pathways. Results indicates that Cu55 (100) will favour *COCOH production over methanol due to small barrier which is key intermediate for finding the efficient catalysts, indicating the possible production of C2 products. Our aim is to find out alloy-based NP catalyst (ex. Cu-Ag etc.) depending on the free energy profile (work already started) having more favorable pathway for C2 compounds.

Keywords: CO2 reduction, alloy catalysts, 111 plane, C2 products

P-21: First Principles Identification of Efficient Single Atom Catalysts for Nitrogen Reduction Reaction

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Abstract:

Chemical ammonia has become an irreplaceable thing in our daily life as its vital role in fertilizer, pharmaceutical and renewable energy. At present, ammonia is produced by the well-known Haber-Bosch process using fossil fuels as the main energy source. Because of large amount of CO_2 is emitted during Haber-Bosch process, the electrosynthesis approach has attracted worldwide research attentions as promising route for achieving green and sustainable ammonia synthesis at ambient conditions. Although exciting advances have been made in NRR field, the electrosynthesis of ammonia is still challenging because of the low ammonia yielding around 0.5% of global ammonia and unsatisfactory Faradaic efficiency mainly deriving from poor catalytic activity of catalysts. As the hydrogen evolution reaction (HER) is the main dominating part for causing poor catalytic activity of catalyst, our main job is finding best catalysts those are NRR favorable over HER. Recent progress in single atom electrocatalyst for producing ammonia has attracted research attentions and become the rising star due to its high selectivity and better Faradaic efficiency. In our research work we are mostly concerned about finding the best single atom catalysts (SACs) using different screening criterion with the help of descriptors like valence electron, d-band center, free energy etc. And for determining the values required for descriptors thus optimizing the catalysts we are using VASP as a computational tool based on density functional theory (DFT).

P-22: Highly textured (Sn, Ga) co-doped ZnO thin films grown by sol-gel route for transparent conductive oxide applications

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Abstract:

(Sn, Ga) co-doped ZnO thin films with varying dopant concentrations were grown on glass substrates by spin-coating a 0.5 M precursor sol synthesized via wet-chemical route. All the films are found to be highly textured oriented along the (0 0 2) lattice plane possessing a ZnO hexagonal wurtzite crystal structure. The improvement in crystallinity (peak intensity) is observed in the doped and co-doped ZnO films. In addition, the (0 0 2) peak position moves towards higher diffraction angle (2θ) owing to smaller ionic sizes of Sn and Ga relative to that of Zn. UV-Visible spectroscopy reveals an improvement in the optical transmittance of the doped and co-doped ZnO films, which is optimum for the 1 at% (Sn, Ga) co-doped film in the wavelength range of 650 – 800 nm. The electrical resistivity measurement exhibits the optimum electrical conductivity for the 1 at% (Sn, Ga) co-doped film. The improved optical transmittance and optimum electrical conductivity of the 1 at% (Sn, Ga) co-doped film support its use for transparent conductive oxide applications.

Keywords: (Sn, Ga) co-doped ZnO thin films; optical transmittance; electrical conductivity

P-23: Green Ammonia Synthesis from Electrochemical Nitrate Reduction on Boron Doped Diamond Electrode

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Abstract:

Electrochemical nitrate reduction is a sustainable alternative method to Haber-Bosch process (Fossil fuel-based energy intensive process) for ammonia synthesis. Large-scale application of electrochemical nitrate reduction has been limited by the lack of catalysts with long-term operational stability and with a high selectivity of nitrate reduction to ammonia by suppressing hydrogen evolution. In this study, we investigated Boron Doped Diamond (BDD) electrode for electrochemical nitrate reduction. Due to the large overpotential towards hydrogen reduction and high corrosion resistance property, BDD electrodes are efficient and highly stable material for the reduction of nitrate ions to ammonia. Prior to the electrochemical experiments, BDD coatings were deposited on the niobium substrate through the hot-filament CVD method. The detailed physical characterization of BDD coating was analyzed through Raman spectroscopy, Scanning electron microscopy, etc. Furthermore, produced ammonia through electrochemical nitrate reduction experiments was quantified by Indophenol method. The achieved Faradaic efficiency was ≈20% at an applied potential of −1.2 V vs Ag/AgCl at pH 7 with a production rate of ≈15.5 mg of ammonia per hour per cm2 of electrode area. Hence, BDD electrodes can be used as an efficient and stable electrode material for sustainable synthesis of ammonia through electrochemical nitrate reduction process.

Keywords: Nitrate Reduction, Boron Doped Diamond (BDD) Electrode, Green Ammonia