SRM UNIVERSITY AP
Andhra Pradesh

# ACCMS Webinars

## 1-44: List of Speakers



**The first-principles phase field method for predicting the microstructure of alloys**

**Prof. Kaoru Ohno**
*Yokohama National University, Japan*



**Multi-scale modelling and theory of structural phase transitions**

**Umesh Wagmare**
*JNCASR*



**High-temperature heat transport in anharmonic systems at the nanoscale**

**Keivan Esfarjani**
*University of Virginia*



**Exploring structure-property relationship of molecular systems via Ab-initio Methods**

**Jer-lai Kuo**
*Institute of Atomic and Molecular Science, Academia Sinica, Taiwan*

@reallygreatsite



**Synergy of computational and experimental approaches in electrochemical energy conversion and storage**

**Bing-Joe Hwang**
*National Taiwan University of Science and Technology*



**Designing the smallest bandgap proper ferroelectric material**

**D. D. Sarma**

*Indian Institute of Science (IISc), Bangalore*



**Recent Advances in Pentagon based 2D materials**

**Qian Wang**

*School of Materials Science and Engineering, CAPT, Peking University, Beijing, China*



**Experimental research on Thermoelectric based oxide thin films: Open question to Computational Materials Sciences**

**Thang Bach Phan**

*Centre for Innovative Materials and Architectures, Vietnam National University, Ho Chi Minh City (VNU-HCM)*



**Extracting Bonds from Bands: COHP and other Chemical-Bonding Tools via LOBSTER**

**Richard Dronskowski**

*RWTH Aachen University*



**Panelist:**

**Kaoru Ohno**

*Yokohama National University*



**Behaviour of Electrons Propagating on 1D Periodic Concave Convex Curved Surface: First Observation of Physical Properties Predicted by Quantum Mechanics of Submanifold**

**Jun Onoe**

*Department of Energy Science and Engineering, Nagoya University, Nagoya, Japan*



**Panelist:**

**Qian Wang**

*School of Materials Science and Engineering, CAPT, Peking University, Beijing, China*



## Hybrid materials from 2D Atomic layer building blocks

**Pulickel M. Ajayan**

*Professor of Materials Science and Nano Engineering, Rice University*



**Panelist:**

**Puru Jena**
*Virginia Commonwealth University*



## Monolayer-protected metal clusters atomically precise, tunable nanomaterials

**Hannu Hakkinen**

*University of Jyvaskyla*



**Panelist:**

**Hui Pan**
*University of Macau*



## Computation, Database and Discovery of 2D Materials

**Yuan Ping Feng**

*National University of Singapore*



**Panelist:**

**Kwang-Ryeol Lee**
*Korea Institute of Science and Technology*



## Electrocatalyst for green hydrogen production design, synthesis and industrial fabrication

**Hui Pan**
*University of Macau*



**Panelist:**

**Thang Bach Phan**
*Centre for Innovative Materials and Architectures, Vietnam National University*



## Materials R&D Data scheme and standard vocabulary

**Kwang-Ryeol Lee**

*Korea Institute of Science and Technology*



**Panelist:**

**G.P Das**

*TCG Centres for Research and Education in Science and Technology*



## Unravelling emergent quantum phenomena from first principles

**Mohammad Saeed Bahramy**

*University of Manchester*



**Panelist:**

**Hiroshi Mizuseki**

*Korea Institute of Science and Technology (KIST) Seoul, Republic of Korea*



## Unravelling emergent quantum phenomena from first principles

**Enge Wang**

*Graduate University of Chinese Academy of Sciences (China)*



**Panelist:**

**Yoshiyuki Kawazoe**

*New Industry Creation Hatchery Centre, Tohoku University*



## Unexpected formation of methane clathrate hydrate in supersaturated methane solution at low pressure

**Vladimir Belosludov**

*Nicolaev institute of inorganic chemistry, Novosibirsk, Russia*



**Panelist:**

**Kaoru Ohno**

*Yokohama National University*



## Toward finite-element modelling of hydrogen isotopes transport for fusion materials from first-principles calculations

**Duc Nguyen Manh**

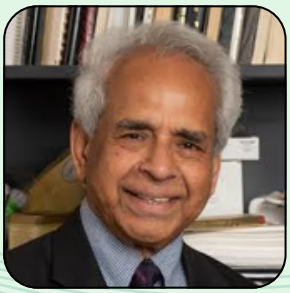
*Culham Centre for Fusion Energy, United Kingdom Atomic Energy Authority, United Kingdom*



**Panelist:**

**Prof. Bing Joe Hwang**

*National Taiwan University of Science and Technology, Taiwan*



## Introduction to Superatomic chemistry and superatom based Materials

**Puru Jena**

*Virginia Commonwealth University*



**Panelist:**

**Prof. Dr. Duc Nguyen Manh**

*Culham Centre for Fusion Energy, United Kingdom Atomic Energy Authority, United Kingdom*



## Synthesis, Applications and Practical Use of Functional Metallo phthalocyanines

**Nagao Kobayashi**

*Tohoku University and Shinshu University*



**Panelist:**

**Prof. Dr. Vannajan Sanghiran Lee**

*University of Malaysia*



## Atomistic configurations in alloying materials: Group III nitrides and high-entropy alloys

**Hiroshi Mizuseki**

*Korea Institute of Science and Technology (KIST) Seoul, Republic of Korea*



**Panelist:**

**Dr. Ryoji Sahara**

*Group Leader in Computational Structural Materials Group, National Institute for Materials Science (NIMS), Japan*



## 2D Nanomaterials for hydrogen storage and electrochemical energy storage: Insights from DFT Simulations

**Brahmananda Chakraborty**

*BARC*



**Panelist:**

**Prof. Talgat Inerbaev**

*L.N. Gumilyov Eurasian National University, Astana, Kazakhstan*



## All electron GW approach for light-element-doped anatase TiO2 using TOMBO

**Ryoji Sahara**

*Tohoku University*



**Panelist:**

**Prof. Jer-Lai Kuo**

*Institute of Atomic and Molecular Sciences, Academia Sinica, Taiwan*



## Fascinating aspects of magnetism in atomically thin two-dimensional materials

**Biplab Sanayal**

*Uppsala University*



**Panelist:**

**Dr. Ryoji Sahara**

*Computational Structural Materials Group, National Institute for Materials Science (NIMS), Japan*



## Off-resonant opt mechanics induced phase transition: Theory and Computational predictions

**Jian Zhou**

*Xi'an Jiaotong University*



**Panelist:**

**Prof. Vannajan Sanghiran Lee**

*Department of Chemistry, Centre of Quantum Information, Science and Technology (QIST), University of Malaya*



## First principles design of effective magnetostriction materials

**Talgat Inerbaev**

*Sobolev Institute of Geology and Mineralogy SB RAS, Novosibirsk 630090, Russia*



**Panelist:**

**Dr. Hiroshi Mizuseki**

*Korea Institute of Science and Technology (KIST), Seoul, Republic of Korea*



## Advances and challenges in DFT-based Design of energy materials for climate change mitigation

**Siriporn Jungsuttiwong**

*Ubon Ratchathani University, Ubon Ratchathani, Thailand*



**Panelist:**

**Prof. Kaito Takahashi**

*Institute of Atomic and Molecular Sciences, Academia Sinica, Taiwan*



## Exploring DNA Dynamics: Energy Landscapes and Molecular Simulations

**Vannajan Sanghiran Lee**

*Department of Chemistry, Universiti Malaya*



**Panelist:**

**Prof. Kaoru Ohno**

*Yokohama National University, Japan*



## New developments in nitride semiconductors focusing on wurtzite structure

**T. Matsuoka**

*Tohoku University*



**Panelist:**

**Prof. Talgat Inervaev**

*L.N. Gumilyov Eurasian National University, Astana, Kazakhstan*



**A guides first-principles calculations tour of HER: Bulk surface, 2D monolayer, and 2D van der Waals heterostructure**

**Darwin Barayang Putungan**

*University of the Philippines Los Banos*



**Panelist:**

**Dr. Do Van Nam**

*Institute for Advanced Studies (PIAS), Phenikaa University, Hanoi, Vietnam*



**Nanomaterials and microscale technologies of engineering muscle tissues.**

**Samad Ahadian**

*NouBio Inc.*



**Panelist:**

**Prof. Vannajan Sanghiran Lee**

*Department of Chemistry, Centre of Quantum Information Science and Technology (QIST) University of Malaya, Malaysia*



**First-principles insights in to magnetic switching: Damping, moment of inertia and charge to spin conversion**

**Satadeep Bhattacharjee**

*Indo Korea Science and Technology Centre, Bangalore*



**Panelist:**

**Prof. G. P. Das**

*TCG-Crest, RISE(Research Institute for Sustainable Energy), India*



**First-principles design of effective magnetostriction materials**

**Masanori Tachikawa**

*Yokohama City University, Japan*



**Panelist:**

**Siriporn Jungsutiwong**

*Ubon Ratchathani University, Ubon Ratchathani, Thailand*



## Charge carriers in Mott insulators — testing the limits of first principles theory

**Hannes Raebiger**

*Yokohama National University*



**Panelist:**

**Tanushri Saha Dasgupta**

*Professor & Director, S. N. Bose National Centre for Basic Sciences, India*



## Localized Molecular orbitals in Mott insulators $GaTa_4Se_8$ and $Nb_3Cl_8$

**Prof. Hongming Weng**

*Director of the Condensed Matter Physics Data Center, Chinese Academy of Sciences*



**Panelist:**

**Prof. Birabar Ranjit Kumar Nanda**

*Professor, IIT, Madras. Department of Physics*



## Quantum Materials by Computation: Challenges & Opportunities

**Prof. Tanusri Saha-Dasgupta**

*Director & Senior Professor*

*S. N. Bose National Centre for Basic Sciences*



**Panelist:**

**Dr. Arkapol Saengdeejing**

*Special Researcher, Research Center for Structural Materials, National Institute for Materials Science, Japan*



## Exploring Transition Metal High Entropy Alloys from First-principles and Machine Learning

**Prof. Ying Chen**

*Professor*

*Tohuku University, Japan*



**Panelist:**

**Dr. Shen Lei**

*Senior Lecturer,*

*National University of Singapore*



## Emergent phenomena exploited at oxide heterointerfaces for unconventional computing

### Prof. Tamalika Banerjee

*Professor & Chair of Spintronics*
*Functional Materials group, Zernike Institute for Advanced Materials, University of Groningen*



**Panelist:**
**Dr. Darwin B. Putungan**
*Institute of Physics, College of Arts and Sciences, University of the Philippines, Los Banos, Philippines*



## AI Physics and Materials Design

### Prof. Xin-gao Gong

*Key laboratory for computational physics (Fudan University), MOE and AI center for physical sciences (Fudan University), Shanghai Education Commission*



**Moderator:**
**Dr. Jung-Hoon Lee**
*Principal Research Scientist*
*Computational Science Research Centre*
*Korea Institute of Science and Technology (KIST)*



## Chiral magnons and anisotropic damping in metallic alter magnets

### Prof. Stefan Blügel

*Quantum Theory of Materials (PGI-1),*
*Peter Grünberg Institute.*
*Institute for Theoretical Physics,*
*RWTH Aachen University.*



**Moderator:**
**Prof. G.P. Das**
*Emeritus Professor,*
*TCG CREST*



## AI-Driven Computational Materials Science: Integrating First-Principles Simulations, HPC, and Materials Informatics

### Prof. Kenta Hongo

*Professor at the Center for Advanced Scientific Computing (CASC), JAIST*



**Moderator:**

**Prof. Ranjit Thapa**

*Professor and Dean - Research*
*SRM University-AP*



## Screening 2D bilayer structures for photocatalytic and ferroelectric applications using high-throughput DFT calculations, materials genome, and machine learning

### Dr Lei Shen

*Senior Lecturer in Department of Mechanical Engineering at National University of Singapore (NUS) and NUS Artificial Intelligence Institute*



**Moderator:**

**Prof. Adisak Boonchun**

*Associate Professor and Chair of Physics*
*Kesetsart University, Thailand*

