SRM UNIVERSITY AP
Andhra Pradesh

ACCMS Webinars

1-35: List of Speakers

The first-principles phase field method for predicting 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

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, HoChiMinh 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

Behavior 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 Center, Tohoku University

Unexpected formation of methane clathrate hydrate in supersatuarated 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

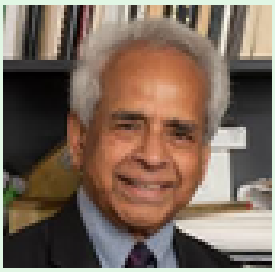
Duc Nguyen Manh

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 Metallophthalocyanines

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, Center of Quantum Information, Science and Technology (QIST), University of Malaya

First principles design of effective magnetostriction materials

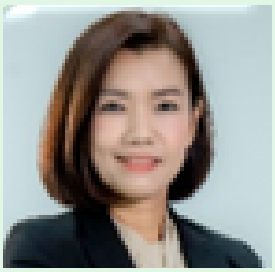
Talgat Inerbaev

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

Panelist:

Dr. Hiroshi Mizuseki

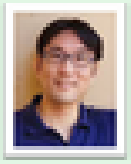
Korea Institute of Science and Technology (KIST), Seoul, Republic of Korea



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, Center 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