

Detailed Program Schedule

21st September, 2016 (Wednesday)²

TOMBO Tutorial (15:00 - 17:00)²

22nd September, 2016 (Thursday)²

Registration Desk Open from 8:00 to 9:00²

Inauguration (9:00 - 9:45)²

Group Photo (9:45 - 10:00)²

Morning Lectures (10:00 - 11:00)²

Tea Break (11:00 - 11:30)³

Parallel Session 1 (11:30 - 13:00) **Oxidation and Battery - I3**

Parallel Session 2 (11:30 - 13:00) **Gas Separation and Solar - I3**

13:00- 14:00 Lunch⁴

Parallel Session 3 (14:00- 15:30) **Catalyst - I and Battery - II4**

Parallel Session 4 (14:00-15:30) **Materials Design and Hydrogen Storage⁵**

15:30 - 15:45 Tea Break⁵

Evening Lectures (15:45 - 18:00)⁵

Cultural Program (18:00 - 19:30)⁶

Welcome Party (19:30 - 21:30)⁶

23rd September, 2016 (Friday)⁶

Registration Desk Open from 8:00 to 9:00⁶

Morning Lectures (9:00 - 11:00)⁶

Tea Break (11:00 - 11:30)⁷

Parallel Session 5 (11:30 - 13:00) **Complex and Structural Materials⁷**

Parallel Session 6 (11:30 - 13:00) **OER, HER, ORR⁷**

13:00 - 14:00 Lunch⁸

Parallel Session 7 (14:00 - 15:30) **2D Materials - I and Strain Effect⁸**

Parallel Session 8 (14:00 - 15:30) **ZnO and Solar - II⁹**

Tea Break (15:30 - 15:45)⁹

Poster Session (15:45 - 18:00)⁹

Banquet Dinner (19:30 - 21:30)⁹

24th September 2016 (Saturday)¹⁰

Session 9 (09:00 - 11:00) **Optoelectronic Devices, 2D Materials - II¹⁰**

Tea Break (11:00 - 11:30)¹⁰

Session 10 (11:30 - 13:00) **Catalyst – II, Hydrogen Storage and SRM University Research Activity¹¹**

Concluding Remarks (13:00 - 13:30)¹¹

Mahabalipuram Tour (13:30 - 19:30)¹¹

ACCMS

Theme Meeting on First Principle Analysis & Experiment: Role in Energy Research

Scientific Program

22nd to 24th September, 2016

Venue: Dr. T. P. Ganesan Auditorium, SRM University, Chennai, India

Time for

Invited=25min talk+5min discussion

Oral=12min talk+3min discussion

21st September, 2016 (Wednesday)

TOMBO Tutorial (15:00 - 17:00)

1. Introduction of ab-initio simulation for explaining materials properties and designing new materials.
2. Importance of all electron formulation in ab-initio simulation and TOMBO project.
3. Hands on training of TOMBO using laptop PC.

Venue: Class Room – **Room No-712, 7th Floor Central Library Building.**

22nd September, 2016 (Thursday)

Registration Desk Open from 8:00 to 9:00

Inauguration (9:00 - 9:45)

Venue: **Main Hall**, Dr. T. P. Ganesan Auditorium.

Group Photo (9:45 - 10:00)

Morning Lectures (10:00 - 11:00)

Venue: **Mini Hall - 1**, Dr. T. P. Ganesan Auditorium.

Chair: **Prof. U. V. Waghmare**

1. (Invited - 1) “How to Predict New Materials such as Penta-graphene with Confidence without Experiments”

Prof. Yoshiyuki Kawazoe

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

2. (Invited - 2) “Computational design of layered 2D materials and their Van der Waals heterostructures”

Prof. G. P. Das

Department of Materials Science, Indian Association for the Cultivation of Science,
Jadavpur, Kolkata, India.

Tea Break (11:00 - 11:30)

Parallel Session 1 (11:30 - 13:00) Oxidation and Battery - I

Venue: **Mini Hall - 1**, Dr. T. P. Ganesan Auditorium (Parallel Session).

Chair: **Prof. A. K. Singh**

1. (Invited - 3) “Strongly Size-Dependent Oxidation and Reduction of Cu Clusters”

Prof. Shobhana Narasimhan

Theoretical Sciences Unit JNCASR Jakkur, Bangalore, India

2. (Oral-1) “Comparative Studies on Structural, Electronic, and Magnetic properties of RT_5 Nano-slabs (R = Y, Ce, Sm and T = Fe, Co, Ni)”

Dr. P. Murugan

CSIR - Central Electrochemical Research Institute, Karaikudi, Tamil Nadu, India.

3. (Oral - 2) “Isolation of pristine Nb_4C_3 MXene from the Nb_4AlC_3 MAX phase”

Dr. Pooja Srivastava

Material Research Centre, Indian Institute of Science, Bangalore, India

4. (Invited - 4) “Bistability switching in CO-oxidation catalysis driven by uni-sized Pt clusters directly bound to Si surface and cluster-size dependence”

Prof. Hisato Yasumatsu

Cluster Research Laboratory, Toyota Technological Institute: in East Tokyo Laboratory,
Genesis Research Institute, Inc., Ichikawa, Chiba, Japan

Parallel Session 2 (11:30 - 13:00) Gas Separation and Solar - I

Venue: **Mini Hall - 2**, Dr. T. P. Ganesan Auditorium (Parallel Session).

Chair: **Prof R. Sahara**

1. (Invited - 5) “Computational materials design for gas separation”

Prof. Hiroshi Mizuseki

Computational Science Research Center, Korea Institute of Science and Technology (KIST), Seoul, Republic of Korea.

2. (Oral - 3) “Thermo-acoustical and computational investigations on green solvent 1-ethyl-3-methylimidazolium tetrafluoroborate with N-methylaniline”

Dr. T. Vijaya Krishna

Department of Physics, Vasireddy Venkatadri Institute of Technology, Guntur, A. P., India

3. (Oral - 4) “An improvement of energy harvesting in organic solar cell using ZnO nanoparticles and nanorods”

Dr. Dang Dinh Long

Faculty of Engineering Physics and Nanotechnology, VNU - University of Engineering and Technology, Hanoi, Vietnam.

4. (Invited - 6) “Mixed Perovskites and IV-VI 2D materials for Photovoltaic Applications”

Prof. Vijay Kumar

Center for Informatics, School of Natural Sciences, Shiv Nadar University, NH91, Tehsil Dadri, Gautam Buddha Nagar, Uttar Pradesh, India.

13:00- 14:00 Lunch

Parallel Session 3 (14:00- 15:30) Catalyst - I and Battery - II

Venue: **Mini Hall - 1**, Dr. T. P. Ganesan Auditorium (Parallel Session).

Chair: **Prof. Chakram Jayanthi**

1. (Invited - 7) “Tailoring properties of low dimensional systems: Support makes the difference”

Dr. Chiranjib Majumder

Bhabha Atomic Research Centre, Mumbai, India.

2. (Oral - 5) “Monolayer BC₂: a high capacity anode material for Li-ion batteries”

Dr. Deya Das

Materials Research Centre, Indian Institute of Science, Bangalore, India.

3. (Oral-6) “Lead-free halide double perovskite Cs₂AgBiX₆ (X=Cl, Br, and I): A first-principles investigation “

Dr. Madhvendra N. Tripathi

Department of Pure & Applied Physics, Guru Ghasidas Vishwavidyalaya (Central University), Koni, Bilaspur, CG, India.

4. (Invited - 8) “Structure and Chemical Activity of Selected Transition Metal and Metal Oxide Catalysts: Theoretical DFT Study”

Prof. Nurbosyn U. Zhanpeisov

Institute for Excellence in Higher Education & Department of Chemistry
Graduate School of Science, Tohoku University, Sendai, Japan

Parallel Session 4 (14:00-15:30) Materials Design and Hydrogen Storage

Venue: **Mini Hall - 2**, Dr. T. P. Ganesan Auditorium (Parallel Session).

Chair: **Prof. Hiroshi Mizuseki**

1. (Invited - 9) “Computational Material Design of Two Dimensional Materials and Their Energy Applications”

Dr. Jer-Lai Kuo

Institute of Atomic and Molecular Science, Academia Sinica, Taipei, Taiwan

1. (Oral - 7) “Temperature, Size and Edge Roughness Dependence of Thermal Conductivity for Vacancy-Defective Monolayer MoS₂”

Dr. Yogeshkumar Sonvane

Department of Applied Physics, Sardar Vallabhbhai National Institute of Technology, Surat, Gujarat, India

2. (Oral - 8) “A DFT Study on the Hydrogen Storage in Ti-Decorated Porous Graphene”

Prof. Manickam Mahendran-O8

Department of Physics, Thiagarajar College of Engineering, Madurai - 625015, India

2. (Invited - 10) “Challenges in exploiting the Kubas Interaction in Hydrogen Storage”

Prof. A. K. Singh

Materials Research Centre, Indian Institute of Science, Bangalore, India.

15:30 - 15:45 Tea Break

Evening Lectures (15:45 - 18:00)

Venue: **Mini Hall - 1**, Dr. T. P. Ganesan Auditorium.

Chair: **Prof. Nguyen Dinh Duc**

1. (Invited - 11) “Tuning Electronic Structure, Topology and Thermoelectric Properties of Metal Chalcogenides: First-principles Simulations”

Prof. U. V. Waghmare

Theoretical Sciences Unit JNCASR Jakkur, Bangalore, India

2. (Invited -13) “Web-based Virtual Lab for the Design of Li Ion Battery Materials: iBat”

Prof. K. R. Lee

Computational Science Center, Korea Institute of Science and Technology, Seoul,
Korea

3. Industry Presentation

Cultural Program (18:00 - 19:30)

Venue: **Main Hall**, Dr. T. P. Ganesan Auditorium.

Welcome Party (19:30 - 21:30)

23rd September, 2016 (Friday)

Registration Desk Open from 8:00 to 9:00

Morning Lectures (9:00 - 11:00)

Venue: **Mini Hall - 1**, Dr. T. P. Ganesan Auditorium

Chair: **Prof. Yoshiyuki Kawazoe**

1. (Invited - 14) “Stable Nanocatalysts and Novel Nanomagnets for Energy and Environment”

Prof. Shiv. Khanna

Department of Physics, Virginia Commonwealth University, Richmond, VA.

2. (Invited - 15) “From Clusters to Crystals: A Bottom-up Design of Energy Materials”

Prof. Puru Jena

Physics Department, Virginia Commonwealth University,
Richmond, VA, USA

3. (Invited - 16) “Nanocomposite materials for energy conversion and storage”

Prof. Nguyen Dinh Duc

Faculty of Engineering Physics and Nanotechnology, VNU - University of Engineering and
Technology, Hanoi, Vietnam.

4. (Invited - 17) "Systematic material design and development for Fuel Cells"

Prof. Takeo Yamaguchi

Tokyo Institute of Technology, Laboratory for Chemistry and Life Science, Japan

Tea Break (11:00 - 11:30)

Parallel Session 5 (11:30 - 13:00) Complex and Structural Materials

Venue: **Mini Hall - 1**, Dr. T. P. Ganesan Auditorium (Parallel Session).

Chair: **Prof. Shiv Khanna**

1. (Invited - 18) "Computational Evaluation of Donor-Bridge-Acceptor (D-B-A) Motifs for High Performance Optoelectronic Device Applications"

Dr. V. Subramanian

Chemical laboratory, CSIR-Central Leather Research Institute, Adyar, Chennai.

2. (Oral - 9) "Ab Initio Modelling of Phase Equilibria in Ti-V, Ti-Nb and Ti-Ta Alloys"

Dr. Ravi Chinnappan

Materials Science Group, Indira Gandhi Centre for Atomic Research, Kalpakkam, India.

3. (Oral - 10) "Phase stability, magnetism and transition temperatures in Ni-Fe-Ga alloys"

Prof. S. S. Chabungbam

Harish-Chandra Research Institute, Allahabad, Uttar Pradesh, India.

4. (Invited - 19) "First principles study of electronic structures and stability in structural materials"

Prof. R. Sahara

National Institute for Materials Science, Tsukuba, Japan.

Parallel Session 6 (11:30 - 13:00) OER, HER, ORR

Venue: **Mini Hall - 2**, Dr. T. P. Ganesan Auditorium (Parallel Session).

Chair: **Prof. Puru Jena**

1. (Invited - 20) " Ab Initio Modelling and Transient Absorption Measurement of Criegee Intermediate Water Vapor Reaction"

Prof. Kaito Takahashi

Institute of Atomic and Molecular Science, Academia Sinica, Taipei, Taiwan

2. (Oral - 11) " Experimental and Theoretical Studies of Bifunctional RGO-CoFe alloy catalyst for OER and ORR reaction"

Dr. Venkataramanan N.S.

Department of Chemistry, School of Chemical and Biotechnology (SCBT), SASTRA University, Thanjavur, India

3. (Oral - 12) "Why Pt skin@PdPt makes stable ORR Electrocatalyst?"

Dr. B. Kakade

SRM Research Institute, SRM University, Kattankulathur , Chennai, India.

4. (Invited - 21) " Structure-Activity Relationship in Graphene Based Electrocatalysts for Hydrogen Evolution Reaction"

Prof. Sang Uck Lee

Department of Applied Chemistry and Department of Bionano Technology, Hanyang University, Korea.

13:00 - 14:00 Lunch

Parallel Session 7 (14:00 - 15:30) 2D Materials - I and Strain Effect

Venue: **Mini Hall - 1**, Dr. T. P. Ganesan Auditorium (Parallel Session).

Chair: **Prof. K. R. Lee**

1. (Invited - 22) "Thermoelectric Properties of the Heterostructures of Graphene and h-BN and related Two-dimensional Nanomaterials: A first-principles approach"

Prof. Sugata Mukherjee

Condensed Matter Physics & Materials Science Department, S.N.Bose National Centre for Basic Sciences, Salt Lake, Kolkata, India.

2. (Invited - 23) "Spin Unrestricted Excited State Relaxation Study of Doped Anatase"

Dr. Talgat Inerbaev

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

3. (Invited - 24) "Strain engineering of carrier mobility in monolayer phosphorene"

Prof. Prasenjit Sen

Harish-Chandra Research Institute, Chhatnag Road, Jhansi, Allahabad, Uttar Pradesh, India.

Parallel Session 8 (14:00 - 15:30) ZnO and Solar - II

Venue: **Mini Hall - 2**, Dr. T. P. Ganesan Auditorium (Parallel Session).

Chair: **Prof. B. Neppolian**

1. (Invited - 25) “Surfing ion-beam fabricated self-organized silicon nanofacets for cold cathode electron emission sites”

Dr. T. Som

Institute of Physics, Sachivalaya Marg, Bhubaneswar, India.

2. (Oral - 13) “Electrodeposited Ni/SiC composite solar selective coating on graphite - Geometry effect on the coatings”

Dr. S. Harinipriya

SRM Research Institute, SRM University, Kattankulathur, Chennai, India.

3. (Oral - 14) “Field-induced doping-mediated tunability in work function of Al-doped ZnO: Kelvin probe force microscopy and first-principle theory”

Dr. Mohit Kumar

SUNAG Laboratory, Institute of Physics, Sachivalaya Marg, Bhubaneswar, India.

4. (Invited - 26) “Investigation of thermal conductivity properties of ZnO nanostructures coated fabric for wearable thermoelectric applications”

Dr. M. Navaneethan

Research Institute of Electronics, Shizuoka University, Hamamatsu, Japan

Tea Break (15:30 - 15:45)

Poster Session (15:45 - 18:00)

Banquet Dinner (19:30 - 21:30)

24th September 2016 (Saturday)

Session 9 (09:00 - 11:00) Optoelectronic Devices, 2D Materials - II

Venue: **Mini Hall - 1**, Dr. T. P. Ganesan Auditorium.

Chair: **Prof. G. P. Das**

1. (Invited - 27) “Understanding and Manipulation of Physical and Chemical Processes in Complex Materials: A first-principles Approach”

Prof. Tanusri Saha Dasgupta

Department of Condensed Matter Physics and Materials Science, S.N. Bose National Centre for Basic Sciences, Salt Lake, Kolkata, India.

2. (Invited - 28) “Function-Oriented Design and Band Gap Engineering of Two-Dimensional Materials for Clean Energy Applications: Hybrid Hexagonal Boron Nitride/Graphene Sheets and Holey Graphene “

Prof. Chakram Jayanthi

Department of Physics and Astronomy, University of Louisville

3. (Oral - 15) “Comprehensively Integrated Environment for advanced MAterials Simulations (CINEMAS)”

Dr. Kapil Gupta

Indo-Korea Science and Technology Centre, Bangalore , India.

4. (Oral - 19) “Metal Decorated BN Linker in MOF as Potential Hydrogen Storage Material”

Dr. T. J. Dhilip Kumar

Department of Chemistry, Indian Institute of Technology Ropar, Rupnagar, India.

5. (Invited - 29) “”

Prof. Ramachandra Rao

IIT Madras, Chennai, Tamil Nadu, India.

Tea Break (11:00 - 11:30)

Session 10 (11:30 - 13:00) Catalyst – II, Hydrogen Storage-II and SRM University Research

Activity

Venue: **Mini Hall - 1**, Dr. T. P. Ganesan Auditorium.

Chair: **Prof. Jer-Lai Kuo, Prof. K. Ramamurthi**

6. (Oral - 17) “Non-regular hexagonal 2D-Dirac carbon: an allotrope of graphene - A First principle study”

Prof. Kombiah Iyakutti

Department of Physics and Nanotechnology, SRM University, Kattankulathur, Tamilnadu-, India.

7. (Oral - 18) “Perovskite solar cell with nontoxic cuprous oxide as hole transporting layer and graphene as transparent electrode: Theoretical study”

Prof. Penchalaiah Palla

Center for Nanotechnology Research, VIT University, Vellore, India.

8. (Invited – 30) “Current Research Activities of IKST and Design of Alloy and Compound Catalysts for Fuel Cell Applications”

Dr. Seung-Cheol Lee

Indo-Korea Science and Technology Center (IKST), Korea Institute of Science and Technology, Bangalore, India.

9. SRM University Presentation

Concluding Remarks (13:00 - 13:30)

Mahabalipuram Tour (13:30 - 19:30)