

# ECS IITMS Student Chapter Inauguration

10 December 2022





# ARCI Industrial Visit

31 December 2022





**INTERNATIONAL CONFERENCE ON ENERGY CONVERSION AND STORAGE (IECS-2023)**  
 With a Pre-Conference Workshop & an Energy Hackathon Contest  
 January 18-20, 2023

**Fastest Finger First Winners (ECS IITM Student Chapter)**

Quiz-1	Quiz-2	Quiz-3
JITHU JOSEPH	SREEJITH OV	GOKUL RAJU
SATYA PRAKASH YADAV	GOKULNATH S	OSHNIK MAURYA
SIDDHARTHA NANDA	VASANTHA A G	KAMAR SAMAN
AKSHAY H	BACHU SRAVAN KUMAR	SUKHJOT KAUR
NIBIN SABARIANAND	EVAN KURIAN	G SRIVIDHYA



# IECS-2023 Fastest Finger First Quiz

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18-20 January 2023





# International Workshop (IWETNGB-2023)

29-30 March 2023





“Electrochemical oxygen intercalation reactions followed up by in situ neutron and synchrotron diffraction at room temperature”

Prof. W. Paulus  
ICGM, Univ. Montpellier, CNRS, ENSCM.



**About The Speaker**

Werner Paulus is full professor (PRCE) at the University of Montpellier (ICGM, UMR 5255) since 04/2011. His scientific interests concern the understanding of solid-state reaction mechanisms mainly of intercalation compounds and more specifically of solid oxygen ion conductors. For structural investigations he is widely using neutron and synchrotron radiation as well as laboratory X-ray diffractometers combined with sophisticated data analysis on complex twinned crystals and by using reconstruction of the scattering density by the Maximum Entropy Method. He has developed specially adapted electrochemical cells, allowing the structural characterisation of reaction intermediates during electrochemically controlled intercalation reactions by in situ neutron and X-ray (synchrotron) diffraction techniques as well as XAFS spectroscopy. He is author of more than 170 publications and 150 communications (international conferences or invited seminar).



Organized by  
ECS IITM STUDENT CHAPTER  
19 APRIL 2023  
11:00 AM IST  
VENUE: CB 310  
DEPT. OF CHEMISTRY

About the talk

Non-stoichiometric oxides with Ruddlesden-Popper structure type and the chemical formula  $A_2B_4O_{10}$  (A = rare earth, B = transition metal) can uptake extra O-atoms on interstitial lattice sites (O<sub>int</sub>). Due to their high mobility even at room temperature, long-range O-ordering up to the sub-mesoscale is observed in several  $A_2B_4O_{10}$  phases, which, together with charge and spin ordering, results into a competitive interplay for the degree of freedom between structural and electronic ordering. Oxygen ordering thus adds an additional degree of freedom affecting charge and spin ordering, entirely absent in the Sr-doped counterpart  $A_2B_6O_{14}$ . Varying the oxygen stoichiometry at ambient temperature by topotactic redox reactions thereby allows to access unusual valence and coordination states. Oxygen doping, which is equivalent to hole doping, gives further on rise to charge ordering phenomena, related to the partial oxidation of the B-cations. Associated to large scale oxygen ordering, this becomes an interesting playground to induce and tune electronic ordering in non-stoichiometric Transition Metal Oxides. It consequently also becomes a promising synthesis tool to install long-range magnetic together with charge ordering. We report here on correlations between structural and electronic ordering phenomena in non-stoichiometric Ruddlesden-Popper type nickelates and cobaltates, carried out on single crystals, using synchrotron and neutron scattering.



# Eminent Lecture Series

19 April 2023





# Workshop on Biosensors

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27 June 2023



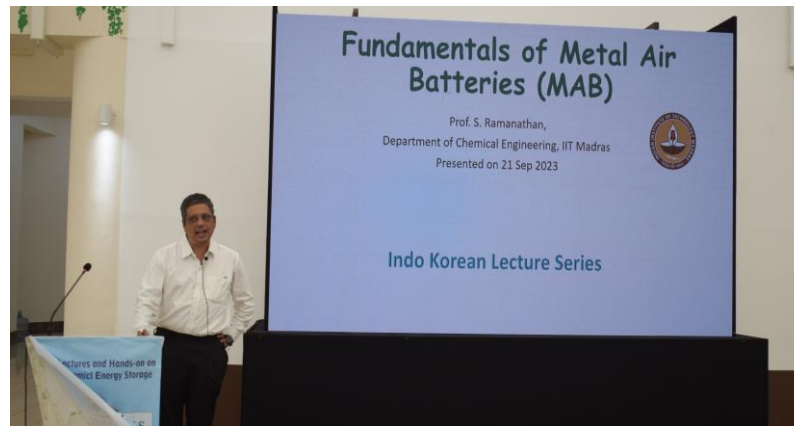


Teacher's Day Celebration

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5 September 2023



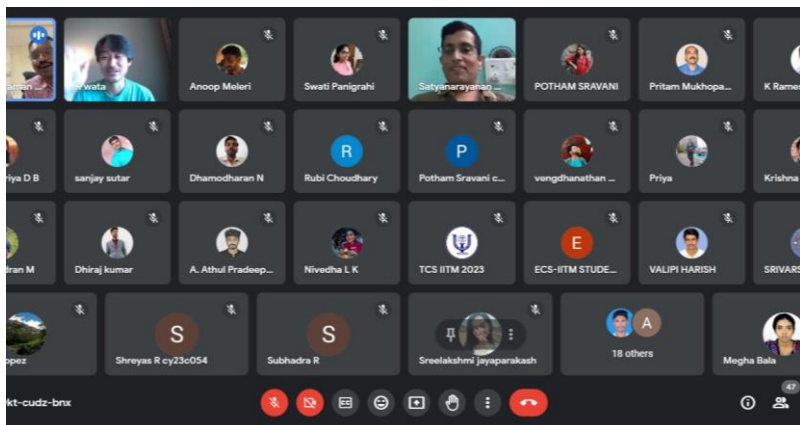
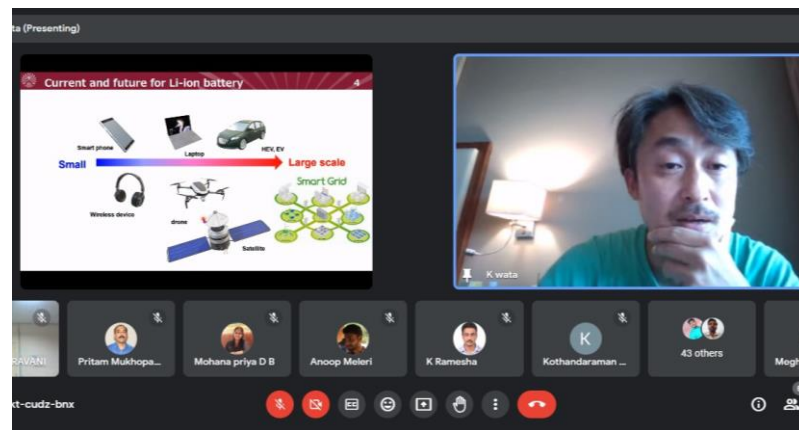
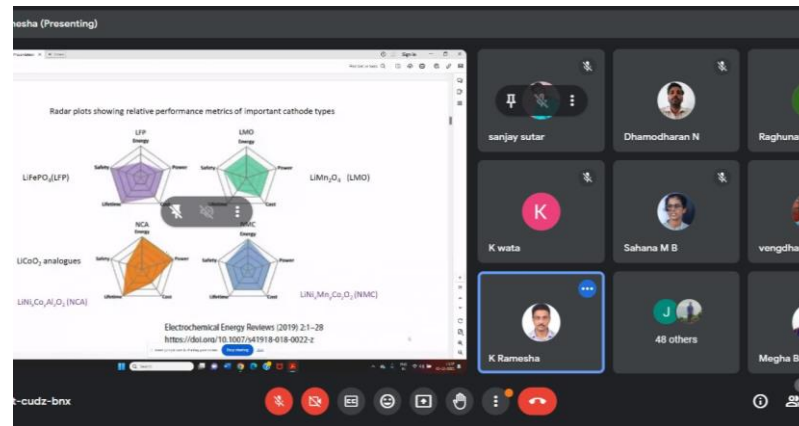


# Indo- Korea Workshop

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20-21 September 2023





**Pre-Energy Summit Workshop**

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**20-21 September 2023**



## “Advanced energy materials for energy conversion device”

ECSI IIT MADRAS Student Chapter



### Dr. Tharamani C. N.

Department of Chemistry, Indian Institute of Technology Ropar, Punjab, India

#### About The Speaker



Dr. Tharamani is an Associate Professor and Head, Department of Chemistry at Indian Institute of Technology (IIT) Ropar. She holds a PhD degree from Bangalore University. Prior to joining IIT Ropar, she spent four years in Germany as senior scientist and postdoctoral fellow at Ruhr University Bochum and a year at University of Saskatchewan, Canada. Her research interests include design and development of various carbonaceous materials, nanomaterials, molecular catalyst with focus on energy conversion and storage, biosensors, in-depth fundamental analysis of the newly designed electrocatalysts towards fuel cells and batteries by various electrochemical, spectroscopic, microscopic and scanning probe techniques (SECM).

Monthly webinar series jointly organized by Electrochemical Society of India - ECSI IITM Student Chapter - Advanced Centre for Energy Storage and Conversion Group @ IITM

26th November 2022 06:00 PM IST

Meeting link: <https://tesol.webex.com/join/j.php?MTID=m2469f786fa93672064cc69f2957247>

## “Beyond Lithium-ion Batteries”

ECSI-IITM-Webinar Series



### Dr. Venkataraman Thangadurai

FRSC (UK), FIAAM, FECS, University of Calgary, Alberta, Canada

#### About The Speaker



Dr. Venkataraman Thangadurai is a full time professor of chemistry at the University of Calgary, Canada. He has more than 230 peer-reviewed papers in journals, his work being cited over 17,000 times with an overall H-index of 59, and was amongst the top 1% of Royal Society of Chemistry (RSC) journals in terms of citations in 2020. He is elected as a Fellow to the Royal Society of Chemistry, UK, fellow of the Electrochemical Society (USA). He received the Keith Laidler Award from the Canadian Chemical Society (CCS) for outstanding early career contributions to physical chemistry and the Award for Research Excellence in Materials Chemistry by the CSC in Canada. Dr. Thangadurai was also appointed as a Scientist and Mentor at the Creative Destruction Lab - Rockies, a non-profit organization that offers programming to enhance the success of scalable, seed-stage science-and technology-based companies. His current research activities include the discovery of novel solid-state batteries, solid oxide fuel cells, electrocatalysis, and electrochemical gas sensors.

Monthly webinar series jointly organized by Electrochemical Society of India - Advanced Centre for Energy Storage and Conversion Group @ IITM

1st October 2022

Meeting link: <https://tesol.webex.com/join/j.php?MTID=m2469f786fa93672064cc69f2957247>

Clean electrochemical energy storage technologies play a vital role in decarbonization. Among the technologies, Li-ion batteries (LIBs) provide higher energy densities (volumetric and gravimetric) than other known secondary batteries. Hence, LIBs are being considered for many applications, including portable electronics, transportation, and grid-scale energy storage. However, commercial LIBs have almost reached their maximum energy densities; their safety also remains a concern. In this talk, approaches to improve the energy density and safety of current LIBs, as well as chemistries beyond lithium, will be presented.

## Computing a Few Electrochemical Properties that can Help us to Identify Whether a 2D Material can be a Promising Anode Material or Not.

ECSI IIT MADRAS Student Chapter



### Dr. Siva Rama Krishna Chaitanya Sharma Yamijala

Department of Chemistry, Indian Institute of Technology Madras, Chennai, India

#### About The Speaker



Yamijala Chaitanya Sharma is an assistant professor in the Chemistry Department, and his expertise lies in the fields of computational chemistry and materials science. He is one of the developers of the quasi-diatribic (QD) PLDM scheme, and he implemented various nonadiabatic dynamics methods such as Ehrenfest, Fewest-Switches Surface-Hopping, QD-PLDM, and MMSI in the DFTB+ package. During his Ph. D. and postdoctoral research career, he excelled in the areas of nonadiabatic dynamics, low-dimensional materials, bio-inorganic chemistry, organic photovoltaics, plasma-assisted catalysis, energy storage materials, and various other interdisciplinary research themes. Prior to his appointment, he did his postdoctoral research in the USA with Prof. Bryan Wong (Department of Chemical Engineering, University of California, Riverside), and with Prof. Pengfei Huo (Department of Chemistry, University of Rochester, New York). Earlier, he earned his M.S. and Ph. D. degrees from the chemistry and physics of materials unit, Jawaharlal Nehru Centre for Advanced Scientific Research (JNCASR, Bangalore, India) under the supervision of Prof. Swapna K. Pati. For a brief period, he had also worked with Prof. S. Balasubramanian (JNCASR).

Monthly webinar series jointly organized by Electrochemical Society of India - ECSI IITM Student Chapter - Advanced Centre for Energy Storage and Conversion Group @ IITM

25th February 2023 05:00 PM IST

Meeting link: <https://tesol.webex.com/join/j.php?MTID=m2469f786fa93672064cc69f2957247>

In this lecture, I will explain the general steps that a computational chemist/materials scientist would go through to find whether a 2D material could be used as an anode material for a specific rechargeable battery or not. To this end, I will use one of our recent publications as a template and show you the results in a step-by-step manner. Ideally, by the end of this workshop lecture, you should be able to know how to compute various physical and electrochemical properties such as the specific charge capacity, open-circuit voltage, Na-atom binding energy, Na-ion diffusion barrier, and so forth, using density functional theory (DFT) calculations. In our work, we considered six cobalt-based anti-MXene materials (Co-anti-MXenes), namely, CoAs, CoB, CoP, CoS, CoSe, and CoSi, and examined their competency as anode materials for NBs. All of these are 2D materials. Our findings suggest that Co-anti-MXenes possess superior specific charge capacities (~390-590 mA h g<sup>-1</sup>) than many well-studied anode materials such as MoS<sub>2</sub> (146 mA h g<sup>-1</sup>), C<sub>2</sub>C (276 mA h g<sup>-1</sup>), expanded graphite (284 mA h g<sup>-1</sup>), and so forth. Moreover, their greater affinity (-0.55 to -1.16 eV) to Na atoms, along with reasonably small diffusion energy barriers (0.32-0.59 eV) and low-average solvation voltages (0.2-0.64 V), suggests that these Co-anti-

## “An overview of CSIR-NALs Solid Oxide Fuel Cell/ Electrolyzer Technology”

ECSI IIT MADRAS Student Chapter



### Dr. S Senthil Kumar

Principal Scientist at National Aerospace Laboratories, Bangalore

#### About The Speaker



Dr. S Senthil Kumar did his Bachelor's in Chemical Engineering from Bharathiar University, Master's from Anna University and Ph.D. from Indian Institute of Science, Bangalore. Worked for many national laboratories such as National Institute of Interdisciplinary Science & Technology, Triruvandrum (2003-2004) as research fellow, Jawaharlal Nehru Aeronautics Research Development, Nagpur as Scientist-I (2004-2005), Central Glass and Ceramic Research Institute, Kolkata (2005-2008) as Scientist and currently, as Principal Scientist at National Aerospace Laboratories, Bangalore (2008- till date) Working in the field of high temperature solid-state electrochemical devices such as solid oxide fuel cell (SOFC) and oxygen sensor. Also, works for space electronics packaging technologies.

Monthly webinar series jointly organized by Electrochemical Society of India - ECSI IITM Student Chapter - Advanced Centre for Energy Storage and Conversion Group @ IITM

28th January 2023 06:00 PM IST

Meeting link: <https://tesol.webex.com/join/j.php?MTID=m2469f786fa93672064cc69f2957247>

Electrical energy storage (EES) systems are mandatory in most renewable power systems. Amongst current EES technologies, EES systems using fuel cells have the highest energy density, longest storage duration, and relatively high power. The storage of hydrogen and derived chemicals, e.g., ammonia and methane, is regarded as the only viable option for electricity storage at a scale of over 10 GWh. Today, the world is looking for sustainable solutions for energy, waste management, and water. In this context, fuel flexibility is considered one of the important criteria for fuel cells and electrolyzers. The ability to accommodate bio-mass derived fuels can provide sustainable solutions for energy and bio-waste management. Technologies based on solid oxide fuel cell electrolyzer can play a vital role in providing viable solutions for the above issues. SOFC converts chemical energy directly to electrical energy and therefore electrical efficiency as high as 60% can be achieved. Further, the higher operating temperature of the SOFC makes it suitable for cogeneration applications whose electrical plus thermal efficiency can reach 80%. The present talk will focus on CSIR-NAL's efforts to develop SOFC/SOEC technologies. In specific, single-cell manufacturing and testing will be highlighted. Also, various cell designs and operating conditions will be discussed in detail.

## “Charge transport at Electrode|Molecule interface”

ECSI-IITM-Webinar Series



### Dr. Veerabhadrarao Kaliginedi

Department of Inorganic and Physical Chemistry (IPC), IISc Bangalore, India

#### About The Speaker



Dr. Veerabhadrarao Kaliginedi is currently working as an assistant professor at the department of Inorganic and Physical Chemistry, IISc Bangalore. He has done his PhD from University of Bern, Switzerland and postdoc from EPFL. His current research activities include the single molecular electronics, spintronics, instrumentation and methodology development, single entity electrochemistry.

Monthly webinar series jointly organized by Electrochemical Society of India - Advanced Centre for Energy Storage and Conversion Group @ IITM

29th October 2022 06:00 PM IST

Meeting link: <https://tesol.webex.com/join/j.php?MTID=m4a28c95164b780a465531c09b09d7e>

Studying the charge transport properties of molecules or nanostructures at single entity level offers huge opportunities to tune structure-property relationships at the nanoscale with a massive range of applications in nanotechnology. In this talk, I will introduce the working principle of measurement techniques (i.e. STM break junctions (STM-BJ), mechanically controllable break junctions (MCBJ)) and data analysis procedures used to extract conductance properties of single molecular junctions. Using the results from several case studies, I will try to demonstrate structure-property correlations of metal/molecule/metal junctions at the single and multi-molecular level.

# ECSI – ECS IITM Monthly Webinar