Invited Lecture
Inter-Disciplinary Explorations in Chemistry (I-DEC 2018)

Computational Modelling of Thermoelectricity, Carrier Mobility and Electro-catalytic Oxygen Reduction Reaction: A Few Examples

Swapan K Pati*
Theoretical Sciences Unit,
School of Advanced Materials (SAMat)
Jawaharlal Nehru Centre for Advanced Scientific Research,
Jakkur Campus, Jakkur, Bangalore 560064
Email: pati@jncasr.ac.in & web: www.jncasr.ac.in/pati/

Abstract:

In recent years, many van der Waals solids, perovskites, spinels etc. exhibit many fold benefits for applications in a number of fields, namely, transparent substrates, field effect transistors, solar cells, thermoelectric materials, active surface for catalysis, rechargeable battery etc, to name a few. In fact, recent experimental advancements on the control over the surface structure of materials has enabled material scientists to tailor the material properties with improved reliability and functionality. We have worked out in detail the thermoelectric behaviour of SnTeSeS systems by co-doping with Ag and In and found the microscopic reason for thermoelectric efficiency to be 1.3 in the case of one of the composition of AgInSnTeSeS [1]. We have also derived relaxation time formulation from complete Boltzmann transport equation and obtained all the parameters from ab-initio density functional theory. Using this formalism, we have calculated charge carrier mobility values and important descriptors. A few cases, such as, trilayer phosphorene and bilayer MoS_2 polytypes will be discussed [2]. We have also been working on Carbon dioxide reduction, Oxygen evolution and reduction reaction by finding stable, cheap and active catalytic surfaces. In this context, I shall discuss the oxygen evolution reaction (OER) on pure and metal doped cobalt oxides, Co_3O_4 and $M_xCo_{3-x}O_4$,(M = Fe, Ni, Cu) surfaces, where the substantial work has been targeted to understand the relation between structure, mechanism, and activity. The activity of the substituted spinels increases relative to that of pure Co_3O_4 and we find that 25 % substitution of Cu in Co_3O_4 has highest electro-catalytic activity with a reduced over-potential value of 0.41 V for OER [3]. If time permits, I shall also discuss developing anode material for Mg-ion rechargeable battery [4].

References and Notes:

References:

1. Biswas, Raju; Roychowdhury, S.; Pati, S K; Biswas, K. "Enhanced Thermoelectricity in Metallic p-type doped SnTe: Role of localised phonons", to be Submitted (2018).
2. Banerjee S.; Pati, S. K. *Nanoscale* **2014**, 6, 13430-13434; *Phys. Chem. Chem. Phys.* **2016**, 18, 16345-16352; S. Banerjee S. et al., *Phys. Chem. Chem. Phys.* **2017**, 19, 21282-21286.
3. Bothra P.; Pati, S K. *ACS Energy Lett.* **2016**, **1,** 858-862; Jana R. et al, *ChemSusChem* **2016**, 9, 2922-2927; Bothra P; Pandey M.; Pati, S. K. *Cat. Sc. & Tech.* 2016, **6**, 6389-6395; Bothra, P.; Pati, S. K. *Nanoscale* 2014, **6**, 6738-6744.
4. Banerjee S.; Pati, S. K. *Chem. Comm.* **2016**, 52, 8381-8384.

Bio-Sketch of Speaker

Dr. Swapan K Pati
Designation: Professor
Department: Theoretical Sciences and School of Advanced Materials
Institute: Jawaharlal Nehru Centre for Advanced Scientific Research
Address: Jakkur Campus, Jakkur, Bangalore 560064
Contact Number: +91-9448560474
e-Mail: pati@jncasr.ac.in & swapan.jnc@gmail.com

Professor Swapan K. Pati obtained his PhD from Indian Institute of Science, Bangalore followed by postdoctoral work at University of California, Davis, and Northwestern University, USA. He joined Theoretical Sciences Unit in JNCASR in November 2000 as an Assistant Professor and in June 2009, he became the full Professor and currently he is the chairman of the same unit. He has received MRSI (2006), CRSI bronze (2007) and BM Birla medals (2008); Swarnajayanthi Fellowship (2007-12), S. S. Bhatnagar award (2010) and The World Academy of Sciences award (2012) in Chemical Sciences. He is a recipient of J. C. Bose national fellowship in 2013 and in 2018. He is an elected fellow of Indian Academy of Sciences (2009), National Academy of Sciences in India (2010), The World Academy of Sciences (2015) and Indian National Science Academy (2018). His research interests include quantum many-body phenomena and quantum chemistry related problems to understand structure property relationships of a large class of systems, ranging from simple molecules to advanced semiconducting device materials. The goal is to design materials for microscopic understanding and application purposes. Some of the current projects in the lab include, frustrated Lewis pair based homogeneous and heterogeneous catalysis, modelling materials for anode/cathode and electrolytes for Li/Na/Mg ion battery, generalized transport phenomena, including heat to current (thermoelectric), light to voltage (photovoltaics) and advanced transistor (FET) devices, phase transitions and new and exotic phases in dipolar Bosonic and Fermionic optical lattice systems. He is also involved in developing new theoretical tools for understanding structure–property correlations.