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Prof. Swapan K Pati
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Theoretical Sciences Unit,
School of Advanced Materials (SAMat),
Jawaharlal Nehru Centre for Advanced
Scientific Research (JNCASR),
Bangalore

On

**“Computational Modeling of a
few Homogeneous and
Heterogeneous Catalytic Reactions”**



3:00 pm, 29 April, 2024



LHC, CR-101

All are cordially welcome

Abstract

Computational Modeling of a few Homogeneous and Heterogeneous Catalytic Reactions

Professor Swapan K Pati

Theoretical Sciences Unit, School of Advanced Materials (SAMat),
Jawaharlal Nehru Centre for Advanced Scientific Research,
Jakkur Campus, Jakkur, Bangalore 560064

E-mail: pati@jncasr.ac.in; swapan.jnc@gmail.com

I shall discuss computational modeling of a few (i) homogeneous catalytic processes, namely, hydrogen activation and hydrogenation of unsaturated systems by Frustrated Lewis Pairs (FLPs) catalysts and (ii) Materials showing electrochemical bifunctional (both oxygen evolution and oxygen reduction) reactions (this can be used as a Zn-air battery) and hydrogen evolution reaction in acidic and at all pH. For the first case, we have worked on several main group elements as frustrated Lewis pairs (FLPs) using a host of Lewis acids, from Boron to Sn^+ to neutral group 14 elements [1]. For the second case, we have collaborated with a few experimental groups to find the bifunctional and water splitting electrocatalytic reactions in several fluoro- & pyro-phosphates and forming heterojunctions and using covalent organic framework [2,3]. In each case, the stability of the hosts, surface types, selectivity, detail mechanism, various reaction intermediates, d-orbital centre, overpotential values and many other quantities relevant for the explanation of experimental data and robust computational prediction would be discussed in details.

References:

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2. K. Sada, R. Gond, N. Bothra, S. K Pati, P. Barpanda, ACS App. Mater. Inter. **14**, 8992 (2022); L. Sharma, N. Bothra, R. Rai, S. K Pati, P. Barpanda, J. Mater. Chem. A **8**, 18651 (2020).
3. S. Dutta, S. K Pati, Cat. Lett. **152**, 3548 (2022); M. Maji, N. Dihingia, S. Dutta, S. Parvin, S. K Pati, S. Bhattacharyya, J. Mater. Chem. A **10**, 24927 (2022).

Swapan K Pati: A Short Biosketch

Professor Swapan K Pati obtained his PhD from Indian Institute of Science, Bangalore, followed by postdoctoral work in Physics at University of California, Davis, and in Chemistry at 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. 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 (TWAS) award (2012). He is a recipient of J. C. Bose national fellowship in 2013, in 2018 and in 2024. He is an elected fellow of Indian Academy of Sciences (2009), National Academy of Sciences in India (2010), TWAS (2015) and Indian National Science Academy (2018). His research interests include quantum many-body phenomena and quantum chemistry related problems to understand the structure property relationships of a large classes of systems, ranging from simple molecules to advanced semiconducting device materials. The goal is to design materials for microscopic understanding and application purposes for the next generation energy and technological devices.

More about him can be found in his homepage and Google Scholar Page:

<http://www.jncasr.ac.in/pati/>

https://scholar.google.co.in/citations?hl=en&user=pGGFotsAAAAJ&view_op=list_works