Short Biodata

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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 as Asst. Prof. in Nov. 2000 and in June 2009, he became a full Professor. He has served as chair of the unit for 2017-2022. Major few awards he has recived are: 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 2023. He is an elected fellow of all the three science academies of India and he is an elected fellow of The World Academy of Sciences. His research interests include quantum many-body phenomena and quantum chemistry related problems to understand the structure property relationships of 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.

Computational Modeling of a few Homogeneous and Heterogeneous Catalytic Reactions

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In this talk, I shall discuss our computational efforts in 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 (OER and ORR; oxygen evolution and oxygen reduction) reactions (this can be used as a Zn-air or Al-air battery) and hydrogen evolution reaction (HER) from water in the acidic medium and at all pH values. For the homogeneous case, we have worked on several main group elements as frustrated Lewis pairs (FLPs) catalysts using a host of Lewis acids, from Boron to Sn^{+} to neutral group 14 elements [1]. For the heterogeneous case, we have worked on finding bifunctional (OER and ORR) electrocatalytic reactions (i) in several transition metal-Nitrogen embedded graphene systems. We have collaborated with an experimental group on several experimentally realized systems, namely (ii) one metal-pyrophosphate and (ii) several metal-fluorophosphates [2]. We also have modelled water splitting electrocatalytic reactions (iv) using covalent organic framework in acidic medium and (v) on an experimentally realized hybrid complex forming heterojunctions at all pH values [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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