Computational Modeling of FLP Catalysts and a few Heterogeneous Catalytic Reactions

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Current research nowadays in materials front always encompasses either creation or storage of renewable energy or development of green chemistry. In this respect, I shall discuss computational modeling of (i) a few homogeneous catalytic processes, namely, hydrogen activation and hydrogenation of unsaturated systems by Frustrated Lewis Pairs (FLPs) catalysts and (ii) 3 fluorophosphates and 1 pyrophosphate showing electrochemical bifunctional (both oxygen evolution and oxygen reduction) reactions (this can be used as a Zn-air battery). For the first case, we have worked on a number 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 an experimental group to find the bifunctional electrocatalytic behaviour in a number of fluoro- and pyro-phosphates [2]. 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 robust prediction and explanation of experimental data would be discussed in detail. If time permits, I shall also discuss our efforts in computationally designing thermoelectric materials for heat to electricity conversion, in particular, about an oxide heterostructure, where due to phonon localization, the thermoelectric efficiency increased many fold in the heterostructure, compared to their individual oxide components [3].

References:

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