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Theoretically Designed Electro- and Photoactivated Earth-Abundant Metal-Based Catalysts for Dihydrogen Generation from Water

Shivnath Mazumder[1]

[1] *Indian Institute of Technology Jammu*

Dihydrogen plays a crucial role in the daunting challenge of replacing fossil fuel-based economy with renewable, clean, and low-cost energy economy. Water splitting by electro- and photo-activated transition metal catalysts has emerged as a viable solution for generation of alternative fuel, H2 gas. However, there are still significant challenges that need to overcome in order to have a commercially viable and low-cost catalyst. The crucial features an efficient and long-lasting catalytic device need to possess are a) unidirectional and kinetically fast multielectron transfer from photosensitizer to the catalytic core, b) robust ligand framework that can sustain different redox states formed in the catalytic cycle, and c) high operational rates by the catalytic core for dihydrogen generation from water. In this regard, several novel Earth-abundant Co-, Ni-, and Cu-based mono- and multimetallic electro-/photocatalysts have been designed via detailed study with Density Functional Theory (DFT). These catalysts can display features like electronic coupling between different metal centers, biomimetic proton relay pathways, and proton-coupled electron transfers to promote their catalytic activity. Moreover, a set of much-needed guiding principles have been provided that can be used by an experimental chemist as a toolbox for synthesis of novel H2 generation catalysts while minimizing the decomposition of the systems.