Computational Roadmap of Emerging Materials: Implications of Piezochromism and Rashba Phenomena

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In this presentation, I would start with the brief introduction of first principles electronic structure calculations in perovskite materials, and how it could be connected to the Computational Screening for achieving highly efficient and stable solar cell materials [1-4]. Next, I will be talking about the fundamentals and possible implications of Rashba phenomena in both hybrid and inorganic perovskite materials [5-7]. The rest of the talk would be devoted to theoretical understanding of piezochromism, where hydrostatic pressure could be employed as an effective tool, giving rise to novel crystal structures and optical properties, while it has proven to be an alternative to chemical pressure. Therefore, new functional materials with intriguing properties can be designed by exerting external pressure and strain. We have also recently [8-10] envisaged the electronic, optical and catalytic properties under the influence of external strain along with the evolution of charge carrier recombination having repercussion on the catalytic activity, mostly hydrogen evolution reaction (HER).

References:

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