Quantum theoretical modeling of smart catalyst design for clean energy and sustainability

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The reliance on fossil fuels has caused major threats to the global climate and environment. As a result, the need for clean energy and environmental sustainability has become a pressing issue. In this regard, hydrogen economy is a transformative vision for a sustainable energy future. Novel catalyst development is important to promote the hydrogen economy for reducing carbon footprint. Such research has been at the forefront and is a key mission for governments worldwide. One of the major roadblocks to implementing the hydrogen economy in terms of technology is the sparse knowledge of physical processes involving the production of hydrogen and its utilization. Hence, there is an active need to explore and understand the atomic and molecular processes occurring at the surfaces/interfaces with hydrogen as a component.

In this presentation, an overview of some of our efforts on critical aspects of catalyst design for hydrogen utilization will be discussed. The research is aimed for energy storage and conversion devices. One such example is the state-of-the-art anion exchange membrane fuel cells (AEMFCs) which offer significant potential for reducing carbon emissions and enhancing energy efficiency [1,2]. The investigations demonstrate a combination of theory and experimental results toward the best catalyst development for hydrogen oxidation reaction (HOR) [1,2]. A set of key descriptors that primarily govern the HOR activity in bi-functional rare-earth transition metal oxides are figured out. The results demonstrate a relatively high HOR performance for the bi-functional system than that of the individual components indicating excellent agreement between the first-principles theory and experimental observations.

References

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