Proton Permeation and Electronic Analysis in 2D Transition Metal Dichalcogenides: A First-Principles Study

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Abstract

With the growing demand for sustainable energy, hydrogen has gained significant attention for its potential as a clean and efficient energy carrier. Proton Exchange Membrane (PEM) Fuel Cells (FCs) represent one of the most advanced and promising options among current hydrogen utilization technologies. Conventionally, PEMFCs employ polymer-based membranes, with Nafion being the most widely used. However, these membranes suffer from considerable performance degradation when exposed to high temperatures and low relative humidity. In addition, PEMFCs performance heavily relies on platinum-based catalysts, which are expensive and scarce**.** These challenges underscore the urgent need to explore novel PEM materials [1, 2]. In this context, 2D materials have emerged as leading contenders, particularly following the breakthrough by Geim's research group, which demonstrated that graphene, though impermeable to gases, exhibits proton conductivity [3].

We will present results concerning the use of Density Functional Theory (DFT) to explore the potential of Transition Metal Dichalcogenides (TMDs) as candidate PEM materials. Proton, lithium, and helium permeation energy barriers are calculated for both pristine and defect-engineered TMDs. In addition, the electronic properties of these materials are examined using charge density plots, charge density difference maps, and Bader charge analysis to understand and explain the observed trends in energy barriers. Figures 1. a, b, and c present an example of these analyses applied to InSe.

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References

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Figures

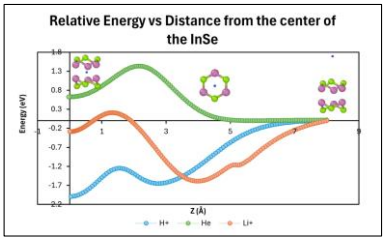

Figure 1.a Energy Profile of H^+, He and Li^+ vs Distance from the center of the monolayer.

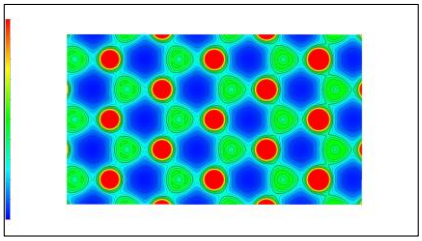

Figure 1.b Charge density Plot of InSe averaged along the perpendicular direction. The contour line in the charge density plots represents 0.05 e/Å³.

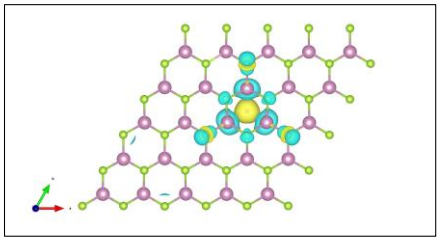

Figure 1.c Charge density difference isosurface plot showing the electronic redistribution upon embedding a proton at the center of a hexagonal ring in a 2D InSe monolayer. Yellow and cyan isosurfaces represent regions of electron accumulation and depletion, respectively, plotted at an isovalue of ±0.0008 e/Å³.