Computational Approaches for Selecting Novel 2D materials for Proton Exchange Membrane Fuel Cells

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Abstract

In the quest for sustainable energy solutions, hydrogen production and utilization play a crucial role. Proton Exchange Membrane Fuel Cells (PEMFCs), known for their high efficiency, low emissions, and adaptability, represent a promising technology in this domain. However, traditional PEMs like Nafion underperform at high temperatures and low humidity, necessitating the exploration of alternative materials [1, 2].

Geim's team has shown that graphene, though impermeable to gases, demonstrates high proton conductivity [3]. This work is focused on investigating proton permeability across a range of two-dimensional (2D) materials by a computational modeling approach, with an initial focus on dichalcogenides. The study involves systematically examining the structures of these materials, engineering specific defects, and evaluating their proton conductivity and selectivity under various conditions [3, 4]. Quantum mechanical simulations and molecular dynamics are employed to model the structural integrity and stability of promising materials, with the goal of advancing the design of high-performance PEMs for hydrogen-based energy solutions.

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References

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Figures

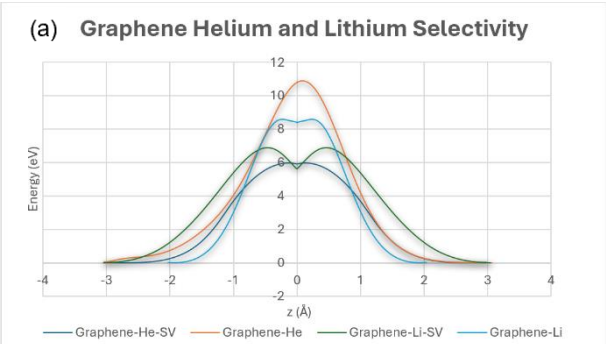

Figure (a): Permeation Energy of He and Li^+ through (1) Pristine Graphene ML, and (2) Graphene ML with single Carbon Vacancy

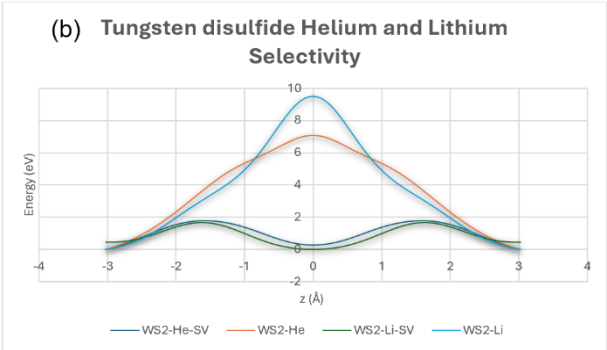

Figure (b): Permeation Energy of He and Li^+ through (1) Pristine WS_2 ML, and (2) WS_2 ML with single Tungsten Vacancy