2D Proton Exchange Membrane Discovery through Atomistic Simulations and Machine Learning

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Abstract

Advancing hydrogen as a sustainable energy source relies on the development of materials with superior proton conductivity for proton exchange membrane (PEM) systems in electrolyzers and fuel cells. These materials are critical for enabling cleaner and more efficient hydrogen production and utilization. PEMs[1] are specialized membranes that allow selective transport of protons (H^+) while blocking electrons and other gas species, making them essential components in hydrogen energy systems.

Previous studies have shown that understanding the energy barriers associated with proton permeation across materials is key to designing efficient proton-conductive membranes. While graphene has been extensively studied, many two-dimensional (2D) materials remain unexplored in terms of their proton permeability. To address this gap, we adopted a synergistic approach combining ab initio molecular dynamics (AIMD) simulations, reactive force field molecular dynamics (ReaxFF MD) and machine learning (ML) techniques to predict and analyze proton permeation barriers across a wide range of non-metallic 2D materials, as illustrated in Figure 1.

We constructed a comprehensive dataset linking proton permeation barriers to nine simple structural and electronic descriptors, including pore diameter, pore size, and atomic electron affinity. This revealed the key physicochemical parameters governing proton transport across 2D materials. Further AIMD simulations evaluated H^+/H_2 selectivity, ultimately identifying 18 promising candidates with low proton permeation barriers. These include well-known 2D materials such as graphene, silicene, and h-BN, affirming the reliability of our screening workflow.

Importantly, several experimentally synthesized but underexplored materials, such as germanene, cubic silicone, TeC, TeCl, GeSe, and Cse, also emerged as promising candidates for PEM applications. For a subset of these materials, including widely studied ones like silicene, we performed ReaxFF MD simulations to assess proton conductivity under varying temperature and humidity conditions. These studies offer critical insights into practical membrane performance under realistic working environments. Most importantly, it provides a powerful strategy for identifying materials that maintain high proton conductivity even under temperatures >100 °C, which is essential to improve the overall efficiency.

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References

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Figures

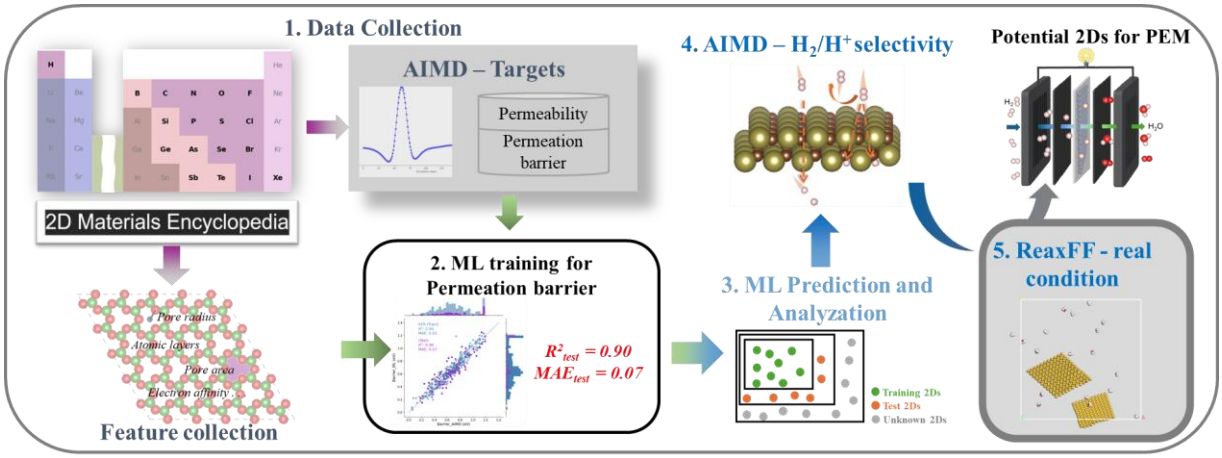

Figure 1: Schematic illustration of discovery materials for PEMs.