Accelerating Hydrogen Fuel Cell Innovation via Machine Learning-Driven Proton Exchange Membrane Discovery

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Abstract (Century Gothic 11)
Advancing hydrogen as a sustainable energy source requires materials with superior proton conductivity for proton exchange membrane (PEM) systems in electrolyzers and fuel cells. These innovations are essential for enabling cleaner and more efficient hydrogen production and utilization. PEM[1] are specialized materials designed to facilitate the flow of protons (H^+) while blocking the passage of electrons and other gases, and they are important in hydrogen electrolyzer or fuel cells. Previous research has proved that understanding the energy barriers involved in proton permeation on 2D materials is essential for designing efficient proton-conductive materials[2]. In addition to graphene, hundreds of two-dimensional materials remain unexplored from a permeability perspective. To address this gap, we employed a synergistic approach combining ab-initio molecular dynamics (AIMD) simulations with Machine Learning (ML) tools as a high-throughput computational method to predict and analyse proton permeation barriers in non-metal 2D materials as shown in Figure 1. We established a permeation barrier dataset that correlates 9 simple structural and electronic properties with proton permeation capacity, shedding light on the key determinants of proton permeation, which includes pore diameter, pore size and atomic electron affinity in modulating proton transport. Further AIMD simulations studied the selectivity for H_2/H^+ with low proton permeation barrier, which screened out 18 promising candidates including widely studied graphene, silicene, and h-BN, supporting the robustness and credibility of predictions. Notably, experimentally synthesized but underexplored materials for PEMs like germanene, cubic silicone, TeC, TeCl, GeSe and CSe, hold significant potential for investigation, while other candidates currently exist only as theoretically stable structures. Therefore, the integration of AIMD and ML accelerates novel materials discovery and interprets physically meaningful rules to bridge theory and experiments, facilitating efficient materials exploration.
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References

[1] Jiao, K. etc. Nature, 595 (2021) 361–369.
[2] Hu, S. etc. Nature, 516 (2014) 227–230.

Figures

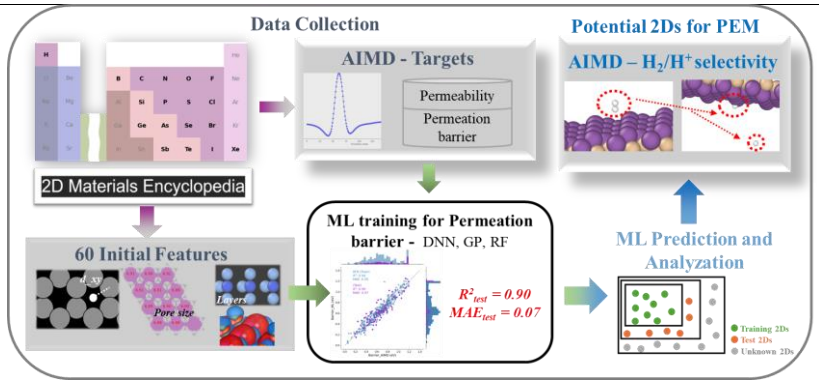

Figure 1: Schematic illustration of discovery materials for PEMs.