Machine Learning-Assisted Prediction of Proton Permeation Barriers in 2D Materials

Yuting Li[1], Daniel Bahamon[1,2], Lourdes F. Vega[1,2]
[1]*Research & Innovation Center for Graphene and 2D Materials (RIC-2D), Chemical and Petroleum Engineering Department, Khalifa University of Science and Technology, PO Box 127788. Abu Dhabi, UAE*
[2]*Research and Innovation Center on CO2 and Hydrogen (RICH), Khalifa University of Science and Technology, PO Box 127788. Abu Dhabi, UAE*

yuting.li@ku.ac.ae, lourdes.vega@ku.ac.ae

Abstract
Proton Exchange Membranes (PEM)[1], often referred to as proton-conductive membranes or proton-conducting electrolytes, 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 a variety of fields, including fuel cells, gas separation and energy storage. The two-dimensional (2D) crystals hold the potential to significantly advance the field of PEM technology, characterized by exceptional molecular permeability and selectivity. Previous research has proved that understanding the energy barriers involved in proton permeation on 2D materials is essential for designing efficient proton-conductive materials[2,3]. This study employs ab-initio molecular dynamics (AIMD) simulations[4] and machine learning (ML) techniques[5] to predict and analyse proton permeation barriers in non-metal two-dimensional (2D) materials as shown in **Figure 1**. Utilizing structures sourced from online databases[6], we calculated permeation barriers on around 500 2D materials through AIMD, thereby establishing a 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, offering insights into the design of advanced 2D materials for proton exchange membranes and fuel cells. The final step involves further assessing the selected potential 2D materials through AIMD simulations to evaluate their selectivity towards hydrogen molecules and protons. This step aims to ensure that the screened 2D materials not only exhibit low proton permeation barriers, but also demonstrate high selectivity for PEM. The integration of AIMD and ML accelerates the discovery of high-performance proton-conducting membranes and provides a deeper understanding of the fundamental mechanisms underlying proton permeation in non-metal 2D materials.
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Figures

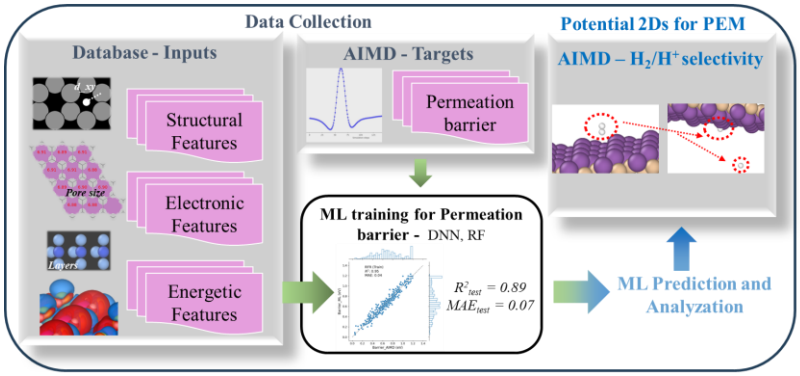

Figure 1: Schematic illustration of predicting of permeation barriers in non-metal 2D Materials using AIMD and ML.