# Exploring proton transport and gas impermeability in 2D Materials: a DFT study

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Abstract
Proton exchange membranes (PEMs) play a crucial role in fuel cells by facilitating proton transport, yet conventional polymer-based membranes suffer from a narrow operating temperature range. Two-dimensional (2D) materials, such as graphene, offer a promising alternative due to their atomic-scale thickness, exceptional mechanical strength, tunable properties, and superior thermal stability [1]. These attributes enable the design of high-performance PEMs with low gas permeability and enhanced proton conductivity, potentially surpassing traditional polymer-based membranes [2].
Beyond graphene, hundreds of 2D-materials remain unexplored for their permeability properties. To bridge this gap, we employed Density Functional Theory (DFT) calculations to systematically screen the permeability of various 2D-material families [3]. Our study focused on monolayer structures from the graphene family (*e.g.*, boron nitride, phosphorene, germanene) and transition metal dichalcogenides (*e.g.*, $MoS_2$, $WSe_2$). Additionally, we examined the influence of atomic doping and defects on transport and permeation selectivity, evaluating a total of 50 2D-structures.
Key insights revealed a strong correlation between proton permeation barriers and fundamental material characteristics, including pore size, interlayer spacing, and atomic electron affinity. Furthermore, simulations assessing $H^+$ selectivity over $Li^+$ ions and helium identified promising, previously unexplored candidates such as germanene, silicene, and $WSe_2$ for PEM applications. These findings also align with recent studies from our group employing machine learning tools for permeability prediction.
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References

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Figures

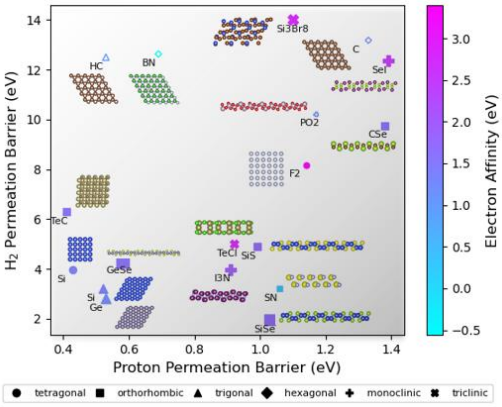


**Figure 1:** Proton and $H_2$ permeation barriers across promising 2D-materials (symbols represent different crystal structures; color scale corresponds to electron affinity in eV).