2D Materials for Clean Energy: From Molecular Design to Scalable Decarbonization Technologies

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Achieving net-zero emissions by 2050—a central objective of the Paris Agreement—requires deep decarbonization of the energy, transportation, and industrial sectors, alongside the rapid development of sustainable materials and technologies.
This presentation highlights how two-dimensional (2D) materials are emerging as enablers of the clean energy transition, focusing on two key areas: hydrogen technologies and carbon capture and utilization (CCUS). Examples from our recent research include graphene-based proton-conductive membranes for fuel cells [1,2] (see Figure 1), graphene oxide–MOF composites for CO_2 capture [3], and heteroatom-doped or nanoparticle-functionalized 2D materials for CO_2 conversion into fuels and chemicals [4]. The talk will demonstrate how computational modeling integrated with machine learning provides molecular-level insights that guide experimental optimization, accelerating the path from material discovery to practical deployment in clean energy systems [5].

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References

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Figures

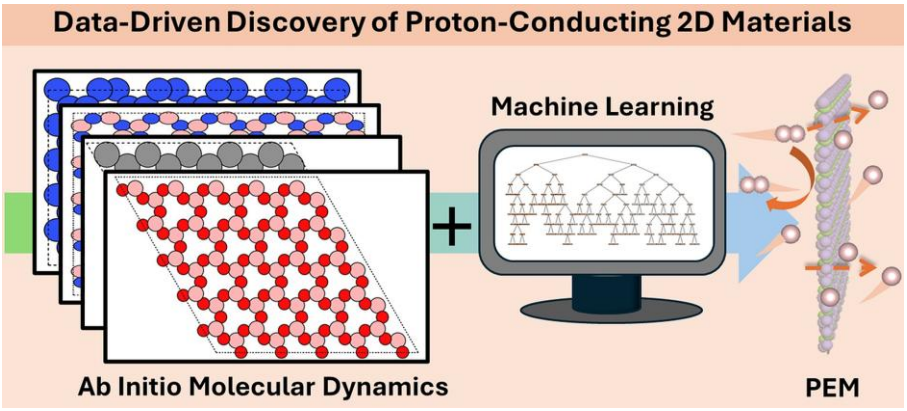

Figure 1: Schematic of the approach for searching proton-conducting 2D membranes for hydrogen applications combining computational modeling with machine learning.