Beyond Functionalization: The Next Frontier of Graphene and 2D Materials for Energy

Lourdes F. Vega[1,2]
Daniel Bahamon[1,2], Yuting Li[1,2], Maryam Khaleel[2], Marcelo Lozada-Hidalgo[3], André Geim[3]
[1]Energy Institute, Khalifa University of Science and Technology, Abu Dhabi, UAE. [2]Research and Innovation Center for Graphene and 2D-Materials (RIC2D), Research and Innovation Center on CO2 and Hydrogen (RICH) and Chemical and Petroleum Engineering Department, Khalifa University of Science and Technology, Abu Dhabi, UAE, [3]Department of Physics and Astronomy and National Graphene Institute, The University of Manchester, Manchester, UK
Contact@E-mail: lourdes.vega@ku.ac.ae

Functionalized graphene and related two-dimensional (2D) materials have become key enablers in energy technologies, spanning electrochemical conversion and storage, catalysis, and separations. While early advances focused on surface functionalization to tune reactivity and transport, the field is now shifting toward integrated multiscale design linking atomic-scale chemistry, mesoscale transport, and device-level performance.

This keynote will address recent progress in the rational design of functionalized graphene and emerging 2D materials for energy applications, combining molecular thermodynamics, high-throughput computation, machine learning, and experimental validation. A central focus is proton-conducting 2D membranes for proton exchange membrane (PEM) technologies, where targeted functionalization enhances proton conductivity, improves chemical stability, and reduces reliance on critical materials[1]. Our recent work[2] demonstrates a machine learning–accelerated discovery framework integrating molecular thermodynamic descriptors with large-scale screening, identifying a new class of proton-conducting 2D membranes beyond graphene, including silicene and germanene derivatives, with exceptional proton selectivity and transport. This provides a predictive route toward next-generation PEMs for hydrogen fuel cells and electrolyzers, currently under investigation in our laboratories.

In addition, electrochemical hydrogenation of graphene will be discussed as a collaborative study with the University of Manchester. This process induces a reversible conductor–insulator transition of interest for logic and memory applications. Our recent results[3] reveal a mechanism governed by proton adsorption competing with hydrogen evolution via an Eley–Rideal pathway. Gibbs free energy analysis reconciles experimental observations and shows kinetics up to six orders of magnitude faster than alternative routes. Nanoscale corrugation and isotope effects further enable tunable control over transition dynamics. The talk concludes with perspectives on AI-driven materials discovery, advanced characterization, and system-level integration for sustainable energy technologies.

Financial support for this project has been provided by the RIC2D Center through project DP001. This research was supported by Khalifa University Research Institute for Energy, Khalifa University of Science and Technology (KU-EI).

References

[1] D Bahamon, Y Li, N Singh, M Khaleel, M Lozada-Hidalgo, LF Vega. Computationally guided design of graphene-like 2D-membranes for selective proton transport in hydrogen fuel cells APL Energy 4, 016102 (2026). https://doi.org/10.1063/5.0300808
[2] Li, Y., Bahamon, D., Lozada-Hidalgo, M., Singh, N., Geim, A. K., & Vega, L. F. *Machine Learning–Accelerated Discovery of Proton-Conducting 2D Materials for Proton Exchange Membranes*. ACS Nano 20, 1, 719–730 (2026). https://doi.org/10.1021/acsnano.5c15161
[3] Soong, YC., Li, H., Fu, Y. et al. Mechanism of the electrochemical hydrogenation of graphene. Nat Commun 16, 10741 (2025). https://doi.org/10.1038/s41467-025-65771-