Graphene and beyond: harnessing the potential of 2D materials for sustainable energy applications

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The increasing concentration of greenhouse gases in the atmosphere, primarily from the energy, transportation, and industrial sectors, and its impact on climate change have driven the adoption of policies aimed at achieving net-zero emissions by 2050, a key objective of the Paris Agreement in 2015. Achieving net-zero emissions requires both the decarbonization of sectors, and the use of materials and technologies that support this transition in a sustainable way. In this sense, the exploration of graphene and other 2D materials has opened new avenues for sustainable energy applications, owing to their exceptional electrical, thermal, and mechanical properties.
Following an overview of the recent applications of these materials in the energy sector, such as in battery technologies [1], photovoltaic cells [2], semiconductors, thermoelectric devices, and supercapacitors [3], the presentation will highlight recent advancements in two clean energy-related applications with significant potential from both fundamental and applied perspectives: hydrogen-related technologies and carbon capture and utilization technologies. Examples will be provided on the use of graphene and other 2D materials as proton conductive membranes for fuel cells [4,5], the combination of graphene oxide with metal organic frameworks (MOFs) and other materials for CO_2 capture [6] and the catalytic activity of graphene and 2D materials when doped with heteroatoms or combined with metal nanoparticles for the conversion of CO_2 into valuable chemicals and fuels. We will emphasize the key role of molecular modeling, including density functional theory combined with machine learning [7] and reactive molecular dynamics play in complementing experimental approaches to optimize the performance of 2D materials in these applications, hence accelerating the deployment of 2D material-based technologies from their fundamental understanding.

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References

[1] L. Shi, T. Zhao, J. Mater. Chem. A, 5 (2017) 3735-3758.
[2] S. Bellani, et al., Chem. Soc. Rev. 50 (2021) 11870-11965
[3] S. W. Bokhari et al., Energy Reports 6 (2020) 2768-2784
[4] S. Hu, *et al*. Nature 516 (2014) 227.
[5] Tong, J., Fu, Y., Domaretskiy, D. et al., Nature 630 (2024) 619–624.
[6] H Zhao, D Bahamon, M Khaleel, LF Vega, Chem. Eng. J. 449 (2022) 137884
[7] Y. Li, *et al*. npj Comput. Mater. 8 (2022) 229.