Multiscale computational modeling for accelerating the understanding and performance of 2D materials for energy applications

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Computational techniques and theoretical models play a key role in establishing the structure–property relationships necessary for understanding and designing materials with novel properties and enhanced performance. These methods range from ab-initio molecular dynamics simulations (AIMD) to density functional theory (DFT), reactive molecular dynamics (ReaxFF MD), classical molecular simulations (MS), kinetic models (KM), coarse-grain models (CG) and process design and optimization (PDO). The increase in computational power together with advanced methods development for calculating properties of materials at different scales has put computational modeling at the forefront of accelerating the materials discovery and design, being an essential tool for this purpose. In recent years, machine learning (ML) combined with AIMD or DFT has gained significant attention in materials design, offering high accuracy with reduced computational costs. The application of these modeling tools combined with advanced experimental techniques is particularly relevant for graphene and 2D materials, as there are several hundreds of 2D materials potential candidates for different applications still to be explored.

In this presentation we will focus on some selected applications of 2D materials related to sustainable energy. Among the different technologies available for reducing greenhouse emissions, green (or low carbon) hydrogen and carbon capture, utilization, and storage (CCUS) have been recently identified by the International Energy Agency as two key technologies to decarbonize the energy and industrial sectors, expected to contribute to 30% to achieving net zero emissions by 2050 [1]. After a general introduction on the need of development efficient materials for energy and the basics on computational modeling, the presentation will focus on the use of combined advanced experimental techniques with computational modeling (and ML) for understanding and improving the performance of 2D materials for selected applications: (1) the development of new proton conducting 2D materials [2] for fuel cells, understanding the effect intense electric fields and nano-scale ripples to increase their catalytic activity [3], where hundreds of materials are explored with the use of ML. This work is done in collaboration with the group of Prof. Sir A. Geim and Dr. M. Lozada-Hidalgo at the University of Manchester through RIC2D, (2) improving the performance and mechanical stability of hybrid adsorbent materials for CO_2 capture, combining graphene oxide (GO) with metal organic frameworks (MOFs) [4] and (3) 2D catalytic materials for CO_2 reduction. We will show how the integration of AIMD and ML not only accelerates the discovery of high-performance proton-conducting membranes but also provides a deeper understanding of the fundamental mechanisms underlying proton permeation in 2D materials. For the case of materials for CO_2 capture, understanding the role of GO through molecular simulations allows optimizing the hybrid composition to improve their performance at the process conditions. Finally, high-throughput screening of 2D materials and their modified versions (doped or functionalized) combining DFT with ML let to identify promising candidates for CO_2 reduction to chemicals and fuels, experimentally validated when possible.

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References

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