Separation of gas through nanoporous graphenes: insights from molecular simulations

Romain Vermorel[1]

[1]*Laboratoire des Fluides Complexes et leurs Ré servoirs, Université de Pau et des Pays de l'Adour, BP 1155, 64013 Pau, France*

In the context of energy transition and carbon dioxide emission reduction, the optimization and development of techniques for separating chemical species in the gas phase is a crucial challenge. Membrane separation and selective adsorption are attractive solutions due to their low energy costs compared to other processes (e.g., cryogenic distillation). In this context, innovative materials such as 2D membranes appear promising: in addition to their advantageous physicochemical properties, they significantly reduce the cost of gas compression. Whether to optimize their performance or guide their design, the theoretical prediction of their transport and separation properties is a goal of great importance.

This presentation summarizes work aimed at clarifying the mechanisms of gas adsorption and diffusion in this type of material, focusing on the example of nanoporous graphene membranes. The proposed methodology relies on molecular simulations to document key mechanisms for inclusion in tractable theoretical models, most often in the form of scaling laws or analytical formulas that highlight the link between performance and membrane structural properties. The case of permeation and separation of small gas molecules is considered, and the importance of taking flexibility into account in graphene molecular models is highlighted.