Contribution ID: **481** Type: **Oral Presentation**

Mechanisms of gas separation through 2D porous graphene membranes : theory and molecular simulations

Thursday, 3 June 2021 19:45 (15 minutes)

In a context of energy transition, the growing share of gas (natural gas, hydrogen, bio-gas) in the energy mix, as well as the need to store CO2 and reduce its emissions, calls for an improvement in gas separation techniques. In this sense, free standing nanoporous graphene is a promising material because it makes it possible to exceed the selectivity to permeance ratio of other membrane materials.

In this study, we use molecular simulations to document the physical mechanisms governing permeation and gas separation through 2D graphene membranes, for different pore sizes and a range of thermodynamic conditions. Our objective is to identify, understand and quantitatively predict the transport properties of gases through these materials.

For pure species, we show that the permeation of a gas molecule consists of two successive steps: the permeation of the membrane plane through the pore and the desorption from the graphene sheet to the bulk. The first step is driven by steric effects in the pore plane. The second stage is the result of a competition between desorption kinetics and surface diffusion along the graphene sheet since an adsorbed molecule can recross the pore or diffuse towards another as long as it does not desorb. On the basis of these observations, we propose a theoretical model that allows us to reproduce the results of the simulations. This model shows that the potential of mean force between a permeating gas molecule and the graphene atoms in the pore region plays a central role.

In addition, we have simulated the separation of gas mixtures (CH4 / CO2, O2 / N2) through various nanoporous graphenes to investigate the selectivity of this type of membrane. Our data show the limits within which the results obtained for pure gases can be used to predict the separation of mixtures.

We believe that these recent results are of interest to help optimise the design of 2D graphene-based membranes, both from the point of view of the geometry or spatial distribution of the pores and their chemical functionalization.

Time Block Preference

Time Block B (14:00-17:00 CET)

References

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Primary authors: Dr VERMOREL, Romain (LFCR, E2S-UPPA); GUO, Juncheng (LFCR, E2S-UPPA, University of Pau and Pays de l'Adour); GALLIERO, Guillaume (Université de Pau et des Pays de l'Adour, France)

Presenter: Dr VERMOREL, Romain (LFCR, E2S-UPPA)

Session Classification: MS13

Track Classification: (MS13) Fluids in Nanoporous Media