

## Efficient molecular design of nanoporous mebranes: the role of intermolecular interactions

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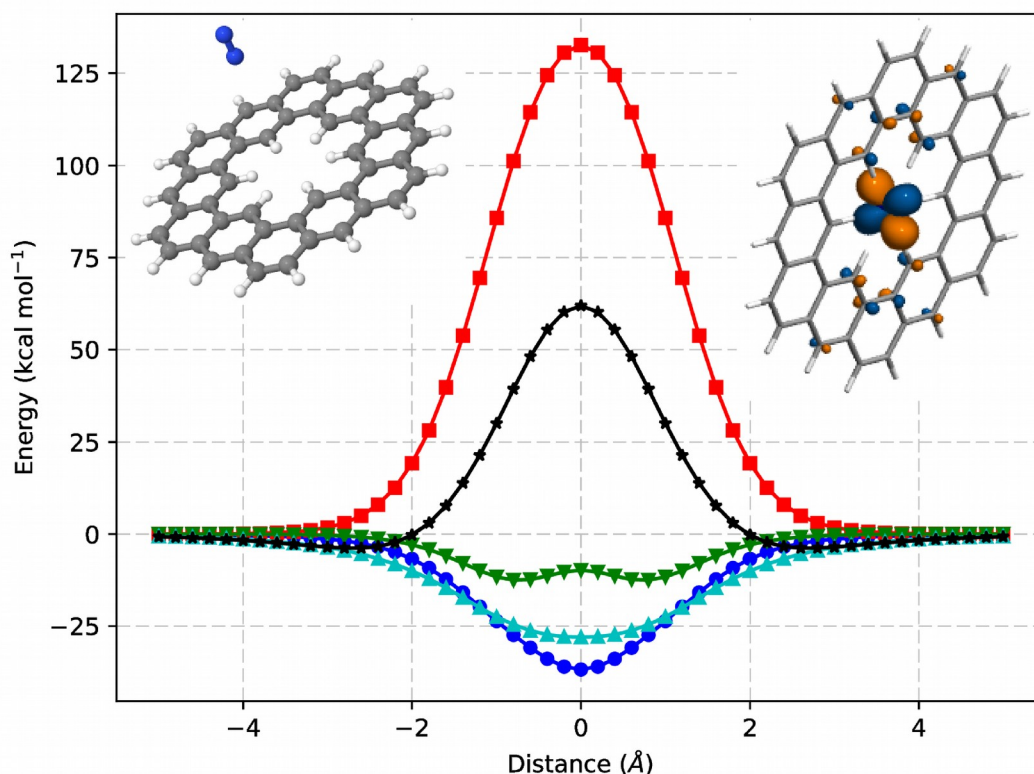
**Abstract:** Gas separation is a subject of relevance for several strategic industrial and chemical processes, encompassing oil refinery and waste gas purification [1,2]. Despite the availability of a wide range of porous membrane structures based on organic polymeric aggregates or silicon derivatives, their efficiency is usually compromised due to their thickness [3]. In this context, graphene-based nanoporous membranes play an important role. While several theoretical studies have already been reported discussing the use of different graphene-based porous structures for the separation of gas molecules [4-7], the interplay between the pore selectivity and specific intermolecular interactions with the approaching system remains to be understood.

The aforementioned question is addressed in the present work by analyzing the diffusion barrier of several gas molecules passing through two carbon-based pores which differs on size and chemical affinity. The potential energy surface (PES) for the interaction is computed by means of the Density Functional Theory, applying various dispersion-corrected exchange-correlation functionals. We were able to verify the importance of the dispersion interaction in order to explain the diffusion barrier and the existence of a minimum well on the PES. A deeper evaluation of the total interaction energy unfolding into its physically meaningful components (electrostatics, exchange, induction and dispersion) is obtained at the Symmetry-Adapted Perturbation Theory [8] level. Our results suggest that, despite the dominance of the exchange interaction due to the steric hindrance, electrostatics and dispersion are key components that could be tuned by chemical modification of the pore structure, leading to an enhancement of the efficiency and selectivity of permeable membranes for gas-separation purposes. Finally, the influence of intermolecular charge-transfer towards the prediction of the diffusion barrier is assessed through the behavior of the induction component and by a detailed analysis of the frontier orbitals of the dimer complex.

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