Grazynes: New membranes for biogas upgrading?

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2D porous membranes are gaining some popularity for selective diffusion processes. For instance, promising results have been achieved in studies on graphene nanostructures [1] and reduced graphene oxides [2]. Here, different nano-engineered grazynes [3], carbon-based materials composed by graphene stripes linked by acetylenic linkages, have been studied as possible membranes to separate methane (CH_4) from carbon dioxide (CO_2) by density functional theory (DFT) and molecular dynamics (MD) computational simulations [4]. The study tackles the process thermodynamics, kinetics, and dynamical aspects associated to the diffusion rates and selectivities in the context of biogas upgrading while comparing to other materials available in the literature. Small adsorption energy values have been obtained for three semi-permeable grazynes, with low diffusion energy barriers which severely reduce as long as the grazyne pore increases. Selectivities towards CO_2 permeation as large as 39 are found at high pressures for [1],[2]{2}-grazyne, closely followed by [1],[2]{(00),2}-grazyne, posing grazynes as excellent membranes for biogas upgrading with clear advantages compared to scrubbing materials in terms of much improved selectivity, continuous workflow and an order of magnitude larger quantity of separated CO_2 per material gram. Present computational simulations reveal that grazynes could be able to upgrade biogas beyond 97 % (v/v) in methane, accomplishing standard worldwide government requirements.

References

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Figures

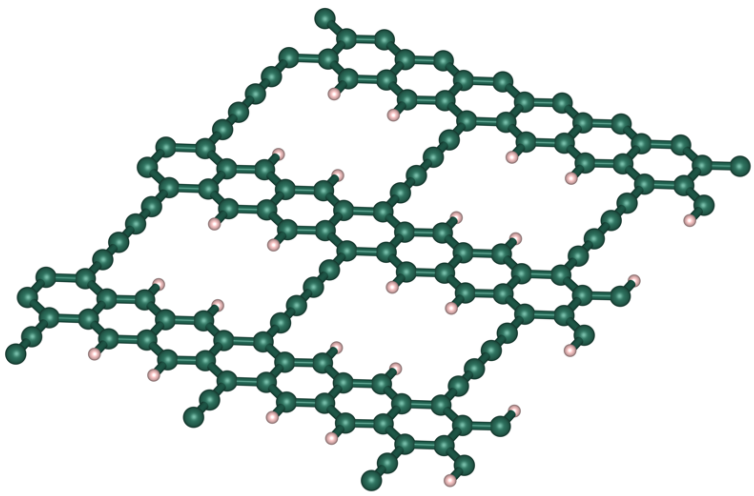

Figure 1: Top view of the [1],[2]{2}-grazyne membrane. Green spheres correspond to C atoms and white spheres denote H atoms.