Theoretical and Physical Chemistry Institute
National Hellenic Research Foundation

Vass. Constantinou 48, Athens

ONLINE LECTURE

"A theoretical study of membranes for gas separation based on one and two layers of nano-porous graphene"

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A theoretical study of membranes for gas separation based on one and two layers of nano-porous graphene

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One of the most promising potential applications of porous graphene is in the field of membranes for gas separation. In this presentation, we include an introductory review showing attempts to overcome a main obstacle in creating useful devices based on a single nano-porous graphene layer. We then present our theoretical work which concerns the permeation of several molecular systems through pores in single layer graphene with the goal to determine the size and type of pores with optimal permeability and selectivity.
Our study is performed at the level of DFT (hybrid-meta GGA functionals). We particularly focused on pores that are created by carbon vacancies and nitrogen doping (pyridinic, pyrrolic defects). We demonstrate that the size of interest for gas separation is 0.5 nm and that pyridinic pores are the most efficient among the types we examined. We also find examples of pores with industrially acceptable permeance that can effectively separate gases. Finally, we turn our attention to pore stacking in bilayer graphene which are studied with atomistic simulations. We show that combinations of pores can be used to enhance/suppress molecular permeability.

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