
# Transmission of Helium through Graphynes' Pores: First Principles Calculations and Quantum Mechanical Simulations

**M. I. Hernández**[a], M. Bartolomei[a], E. Carmona-Novillo[a], J. Campos-Martínez[a], F. Pirani[b] and G. Giorgi[c]

[a] Dpto. de Física Atómica, Molecular y de Agregados, Instituto de Física Fundamental, C.S.I.C., Serrano 123, Madrid 28006, Spain
[b] Dipartimento di Chimica, Biologia e Biotecnologie, Università di Perugia, Perugia, Italy
[c] Department of Chemical System Engineering, School of Engineering, U. Tokyo, Tokyo, Japan

Graphynes are novel two-dimensional carbon-based materials that exhibit regular and uniformly distributed subnanometer pores (FIG. 1). These features make them very promising materials for gas filtration applications at the molecular level[1]. Our goal is to study the interaction and dynamics of transmission of small molecules through graphynes' pores from first principles quantum mechanics calculations.

We will report on a recent work[2] focused on the properties of graphdiyne (whose molecular precursor is shown in the center of FIG. 1) as a filter of $^4$He from $CH_4$, and of $^3$He from $^4$He. Accurate electronic structure calculations have served to obtain a new force field suitable for molecular dynamics simulations. In particular, one-dimensional (1D) quantum mechanical transmission probabilities show a favorable $^3$He/$^4$He selectivity at low temperature. More recently, we are studying the role of the in-pore degrees of freedom and their eventual anharmonicity by means of the transition state theory[3]. Finally, we will present preliminary 3D time-dependent wave-packet simulations of the transmission of the two He isotopes through the graphynes' pores.

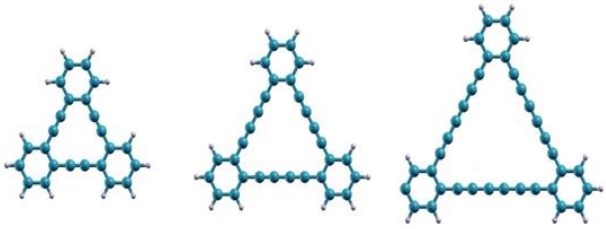

FIG. 1: Annulenic molecular precursors of graphyne, graphdiyine and graphtriyne.

[1] S. W. Cranford and M. J. Buehler, *Nanoscale* **4**, 4587 (2012)
[2] M. Bartolomei, E. Carmona-Novillo, M. I. Hernández, J. Campos-Martínez, F. Pirani, G. Giorgi, *J. Phys. Chem. C* **118**, 29966 (2014).
[3] M. Hankel et al., *Phys Chem. Chem. Phys.* **13**, 7834 (2011)