



CECAM WORKSHOP “Modeling dilute matter in ultracold conditions: from quantum structure to dynamics and reactivity”

José Campos-Martínez, M. Bartolomei, M. I. Hernández

j.campos.martinez@iff.csic.es

Instituto de Física Fundamental (IFF-CSIC)
Serrano 123, E-28006 Madrid (SPAIN).

"Quantum sieving of Helium isotopes through two-dimensional membranes"

Two-dimensional (2D) membranes are attractive materials with countless applications both in basic research or applied technologies[1]. One of such applications concerns the separation of different atomic or molecular species when the 2D layer have nanopores of an adequate size[2]. There exists also possibilities for isotopic separation when one considers quantum effects associated to the size of the nanopore or low temperature in the system. We will present results on the separation of $^3\text{He}/^4\text{He}$ isotopes with different types of membranes and nanopores[3,4] through rigorous 3D wave packet calculations[5] and intermolecular potentials[6] based on high-level ab-initio calculations which are fit to an analytical formula. We will discuss the different features shown by different materials, the relative importance of quantum effects, or new ways of including more degrees of freedom yet preserving an appropriate description of quantum phenomena.

[1].- Tan, Ch. *Et al. Chem. Rev*, 117, 6225 (2017).

[2].- a) Huang C. *et al.*, *Chem. Rev.*, 118, 7744 (2018), b) Kim S, *Angew. Chem. Int. Ed.*, 58, 17512 (2019) c) Bartolomei, M. *et al. J. Phys. Chem. Lett.* (2014), 5, 751–755.

[3].- Moreno, C. *et al. Science* (2018), 360, 199–203.

[4].- Hernández M.I., *Nanomaterials*, 11, 73, 2021.

[5]- Gijón, A. *et al. The Journal of Physical Chemistry C* (2017), 121, 19751–19757.

[6]-Bartolomei, M. *et al. J. Phys. Chem. C* (2014), 118, 29966–29972.