Three-Dimensional Wave-Packet Calculations of the Transmission of He Isotopes through Graphynes Membranes

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Graphynes are novel two-dimensional carbon-based materials that exhibit regular and uniformly distributed sub-nanometer pores [1]. These features make them very promising materials for gas filtration applications at the molecular level [2]. In this contribution, we will present a new three-dimensional time-dependent wave-packet approach for the calculation of the probabilities for the transmission of atoms through the pores of a two-dimensional membrane. The method is applied to the passage of ^{3}He and ^{4}He through of graphdiyne and graphtriyne, two members of the family of γ-graphynes. The interaction between the He atoms with the membrane is represented by a new force field based on accurate electronic structure calculations [3]. We are particularly interested in studying the interplay between tunneling and zero point energy effects in the ^{3}He/^{4}He selectivity (isotopic separation) as a function of the temperature. In this way, the results of the TSWP calculations will be discussed in comparison with a previous study based on tunneling-corrected transition state theory [4].

References

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