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【445】Stacked sheets of porous 2D carbon materials for chiral selection

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Recently, stacked sheets of nanoporous graphene have been suggested for the separation of racemic mixtures with respect to molecular chirality. Different pore arrangements lead to different barrier heights for the two enantiomers of a given molecule. We are investigating the performance of these membranes via a combination of a recent force-field ansatz of the Grimme group with nudged-elastic-band calculations. First, the energy barriers for methane and nitrogen are calculated for different pore sizes and arrangements. Probabilities for propagation are studied via molecular dynamics and compared to predictions based on transition state theory. Second, we investigate chiral separation tendencies in the case of D- and L-Leucine.

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