612c Quantum Sieving of Hydrogen Isotopes in Carbon Nanotubes

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The difference in the zero point energy of hydrogen isotopes adsorbed in narrow carbon nanotubes could be used to separate them with great efficiency. Using Path Integral Monte Carlo simulations we calculate the adsorption isotherm of hydrogen isotopes at 20 K and the selectivities than can be expected in various types of carbon nanotubes, as well as its dependence on the potential model. Our results indicate that in the narrowest tube we have simulated - the (3,6) - one could expect selectivities as high as 10^{10}. The selectivity drops dramatically if larger tubes are considered, being of order 10 in the (6,6) and (10,10) tubes. We take into account the diatomic structure of the hydrogen molecule and show that the explicit treatment of the rotational degrees of freedom is necessary in order to calculate the precise value of the selectivity.

We develop an approximate method to calculate the selectivity, according to which it can be written as the product of a factor referring to the center of mass degrees of freedom and a factor describing the coupling between translational and rotational motions. These two factors are of the same order (around 10^5) in the case of the (3,6) tube.