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Quantum Tunneling of Thermal Protons Through Pristine Graphene IGOR POLTAVSKYI, Physics and Materials Science Research Unit, University of Luxembourg, Luxembourg, MAJID MORTAZAVI, Fritz-Haber-Institut der Max-Planck-Gesellschaft, Berlin, Germany, ALEXANDRE TKATCHENKO, Physics and Materials Science Research Unit, University of Luxembourg, Luxembourg — Atomically thin two-dimensional materials such as graphene and hexagonal boron nitride have recently been found to exhibit appreciable permeability to thermal protons, making these materials emerging candidates for separation technologies [S. Hu *et al.*, Nature 516, 227 (2014); M. Lozada-Hidalgo *et al.*, Science 351, 68 (2016).]. These remarkable findings remain unexplained by density-functional electronic structure calculations, which instead yield Arrhenius activation energies that exceed by $\sim$1.0 eV those found in experiments. Here we demonstrate that the thermal proton transfer through pristine graphene is driven by nuclear quantum effects, which substantially reduce the value of Arrhenius activation energy by up to 1.0 eV compared to the results of classical molecular dynamics. We show that an account for pre-exponential factors in the Arrhenius equation (entropic effects) is crucial in order to reproduce the observed isotope effect. Due to different delocalization of protons and deuterons these factors differ by more than seven orders of magnitude. Our findings offer new insights for controlling the underlying quantum ion transport mechanisms in nanostructured separation membranes.

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