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Multiscale Modeling of Small Molecules in Zeolite-4A

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Confinement within the nanoscale pores of a zeolite strongly modifies the behavior of small molecules such as water, ammonia, and the ammonium ion. Typical of many such interesting and important problems, realistic modeling of this phenomena requires simultaneously capturing the detailed behavior of chemical bonds and the possibility of collective dynamics occurring in a complex unit cell (672 atoms in the case of Zeolite-4A). Classical simulations alone cannot reliably model the breaking and formation of chemical bonds, while quantum methods alone are incapable of treating the extended length and time scales characteristic of complex dynamics. We report results from a hybrid approach combing first-principles electronic structure calculations, classical molecular dynamics and Monte Carlo simulations, and a recently developed model in which a small region treated with the Kohn-Sham density functional theory is embedded within a larger system represented by classical potentials.