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A chemical reaction in the worst possible solvent? Quantum modeling of NaCl in helium nanodroplets

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Helium nanodroplets provide an extremely cold and inert solvent that can embed most (but not all) atoms, ions, or molecules. Long-range electron transfer reactions inside helium droplets were suggested in experiments on alkali dimers interacting with fullerenes solvated inside helium nanodroplets [Renzler et al., J. Chem. Phys. **145**, 181101 (2016)]. In the present work, we present preliminary computational effort towards the atomistic modeling of such processes, focusing on the simpler case of an archetypal chemical reaction involving electron transfer, namely the formation of the ionic bond in the NaCl diatomic, in the presence of a helium nanodroplet. A simple but realistic model for the chemical interaction was constructed based on the empirical valence-bond approach and appropriate polarizable potentials for the solvent, time-dependent simulations accounting for nuclear delocalization being carried out in the framework of ring-polymer molecular dynamics.

Two types of computational experiments were conducted, in which neutral Na and Cl atoms are brought closer from one another and made to react either through collision processes, or via the sequential evaporation of the droplet. In both cases, we find evidence for a significant influence of nuclear quantum effects, not only acting on the solvent itself but also affecting the NaCl molecule that forms in the outer regions of the droplet.