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Reptation Quantum Monte Carlo Calculation of Charge Transfer in The Na-Cl Dimer YI YAO, YOSUKE KANAI, Department of Chemistry University of North Carolina at Chapel Hill — Reptation Quantum Monte Carlo (QMC) calculations are performed to describe the charge transfer behavior in a NaCl dimer. Influence of fixed node approximation on the charge transfer was examined by obtaining electron density via reputation QMC. We employ Slater-Jastrow wavefunction as the trial wavefunction, and the fermion nodes are obtained from single particle orbitals of Hartree-Fock and Density Functional Theory (DFT) with several exchange-correlation approximations. We will discuss our QMC results together with DFT calculations to give insights into observed dependence of the charge transfer behavior on the fixed-node approximation.

Yi Yao
Department of Chemistry University of North Carolina at Chapel Hill

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