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**Role of Inter-molecular Charge Transfer in Simulating Concentration Dependent Water Diffusivity of Aqueous Salt Solutions** YI YAO, MAX BERKOWITZ, YOSUKE KANAI, Univ of NC - Chapel Hill — The translational diffusivity of water in solutions of alkali halide salts depends on the identity of ions, exhibiting dramatically different behavior even in solutions of similar salts of NaCl and KCl. The water diffusion coefficient decreases as the salt concentration increases in NaCl. Yet, in KCl solution it slightly increases and remains above bulk value as salt concentration increases. Previous classical molecular dynamics simulations have failed to describe this important behavior even with polarizable models. Here we show that the missing physical effect in previous simulations was charge transfer; its inclusion produces results in a quantitative agreement with experiments. We found that the concentration-dependent diffusivity reflects the importance of many-body effects among the water molecules when the ions are present. Explicit inclusion of charge transfer allows us to model accurately the difference in the concentration-dependent water diffusivity between $Na^+$ and $K^+$ ions in simulations, and it is likely to impact modeling of a wide range of systems.

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