Abstract Submitted
for the MAR17 Meeting of
The American Physical Society

Cl- solution studied by *ab initio* molecular dynamics considering nuclear quantum effect on proton[1] ZHAORU SUN, MOHAN CHEN, XIFAN WU, Temple University — The H-bond structure perturbed by solvated ions of the Hofmeister series is a topic of great interest in many biological, biochemical and electrochemical process. In classical *ab initio* molecular dynamics (AIMD) simulations, the Cl- , a representative ion, does not significantly affect the structure of water for dilute solution with salt concentration below 1M. Recently, it is found that nuclear quantum effect (NQE) has significant influence on the hydrogen bond in pure water by softening the H-bond. By considering the NQE on proton in both dilute Cl- solution and pure liquid water using path integral molecular dynamics with colored noise thermostat, we find that the oxygen-oxygen radial distribution functions in Cl- solution is over-structured than that in pure water, indicating that the hydrogen bond in Cl- solution becomes stronger. We will validate our finding by the analysis of solvation structure change, Wannier center distribution and dipole moment of water. Our work shows that NQE cannot be neglected for the hydrogen bond network in Hofmeister ion solutions.

[1]DMR-1552287, DESC0012575

Zhaoru Sun
Temple Univ

Date submitted: 11 Nov 2016 Electronic form version 1.4