Abstract Submitted
for the MAR17 Meeting of
The American Physical Society

First-Principles Molecular Dynamics Simulations of NaCl in Water: Performance of Advanced Exchange-Correlation Approximations in Density Functional Theory YI YAO, YOSUKE KANAI, UNC-Chapel Hill — Our ability to correctly model the association of oppositely charged ions in water is fundamental in physical chemistry and essential to various technological and biological applications of molecular dynamics (MD) simulations. MD simulations using classical force fields often show strong clustering of NaCl in the aqueous ionic solutions as a consequence of a deep contact pair minimum in the potential of mean force (PMF) curve. First-Principles Molecular Dynamics (FPMD) based on Density functional theory (DFT) with the popular PBE exchange-correlation approximation, on the other hand, show a different result with a shallow contact pair minimum in the PMF. We employed two of most promising exchange-correlation approximations, ωB97xv by Mardiorossian and Head-Gordon (1) and SCAN by Sun, Ruzsinszky and Perdew (2), to examine the PMF using FPMD simulations. ωB97xv is highly empirically and optimized in the space of range-separated hybrid functional with a dispersion correction while SCAN is the most recent meta-GGA functional that is constructed by satisfying various known conditions in well-defined physical limits. We will discuss our findings for PMF, charge transfer, water dipoles, etc. (1) Mardirossian, Narbe, and Martin Head-Gordon. *Physical Chemistry Chemical Physics* 16.21 (2014): 9904-9924. (2) Sun, Jianwei, Adrienn Ruzsinszky, and John P. Perdew. *Physical review letters* 115.3 (2015): 036402.

Yi Yao
UNC-Chapel Hill

Date submitted: 09 Nov 2016 Electronic form version 1.4