Supporting Information to:
Similarities and Differences between Potassium and Ammonium Ions in Liquid Water: A First-Principles Study

Fikret Aydin,† Cheng Zhan,† Cody Ritt,† Razi Epsztein,‡¶ Menachem Elimelech,‡ Eric Schwegler,† and Tuan Anh Pham*†

†Quantum Simulations Group, Materials Science Division, Lawrence Livermore National Laboratory, Livermore, CA 94550, USA
‡Department of Chemical and Environmental Engineering, Yale University, New Haven, CT, 06520-8286, USA
¶Faculty of Civil and Environmental Engineering, Technion-Israel Institute of Technology, Technion City, Haifa 32000, Israel

E-mail: pham16@llnl.gov
Figure S1: Nitrogen–oxygen radial distribution functions computed for solvated \( \text{NH}_4^+ \) in liquid water. Black and red lines indicate results obtained from 20 ps NVT simulations using Bussi-Donadio-Parrinello (BDP) and velocity scaling thermostats, respectively.