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

Fikret Aydin,<sup>†</sup> Cheng Zhan,<sup>†</sup> Cody Ritt,<sup>‡</sup> Razi Epsztein,<sup>‡,¶</sup> Menachem

Elimelech,<sup>‡</sup> Eric Schwegler,<sup>†</sup> and Tuan Anh Pham<sup>\*,†</sup>

†Quantum Simulations Group, Materials Science Division, Lawrence Livermore National Laboratory, Livermore, CA 94550, USA

<sup>‡</sup>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

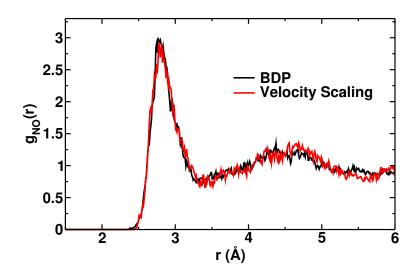


Figure S1: Nitrogen-oxygen radial distribution functions computed for solvated  $NH_4^+$  in liquid water. Black and red lines indicate results obtained from 20 ps NVT simulations using Bussi-Donadio-Parrinello (BDP) and velocity scaling thermostats, respectively.