Supporting Information: 2D nanoconfinement distorts the solvation structure of hydroxide but not of hydronium

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1 MLIAP Validation

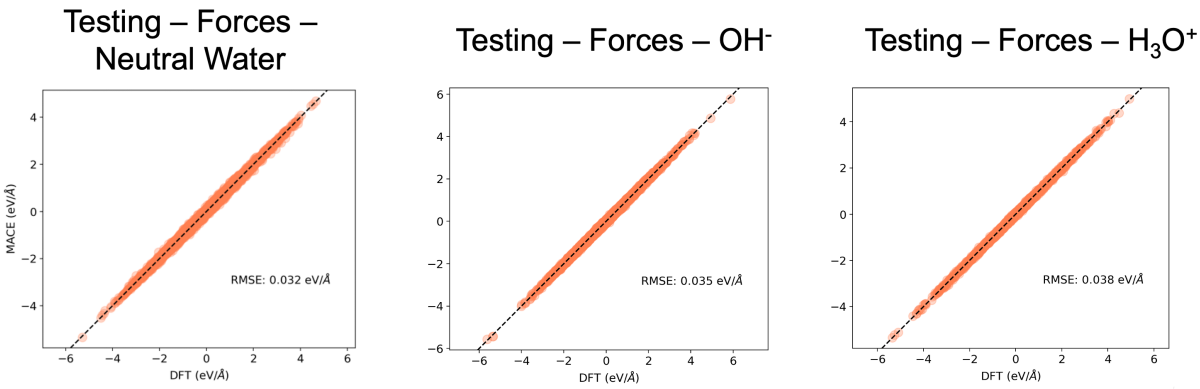

Figure S1: Parity plots of the forces from 105 total frames not included in the training set from all systems sampled in training. Hydronium and hydroxide parity plots are for frames with either ion present in the confined water or bulk system.

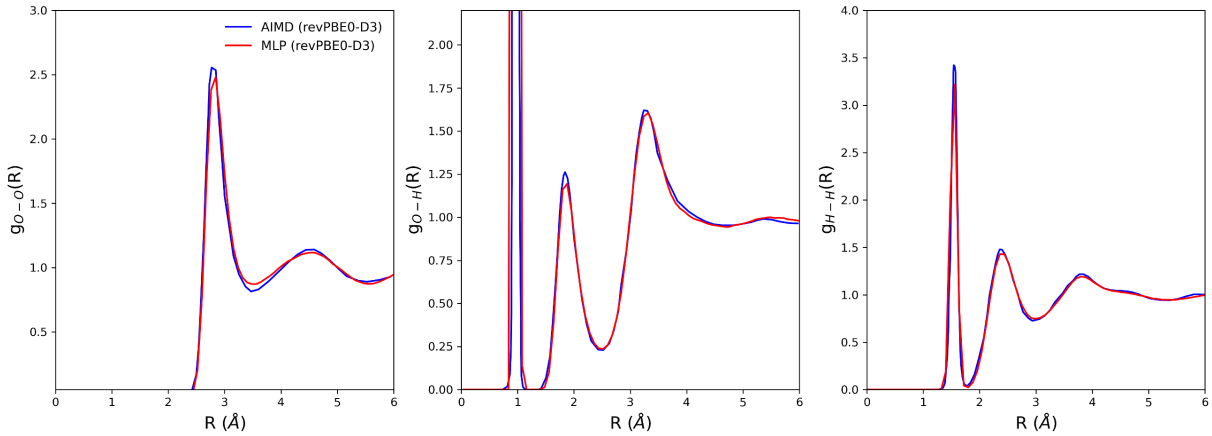

Figure S2: Radial distribution functions of OH, OO, and OH of bulk liquid water using the trained MLIAP compared to a short 10 ps AIMD run for bulk liquid water.

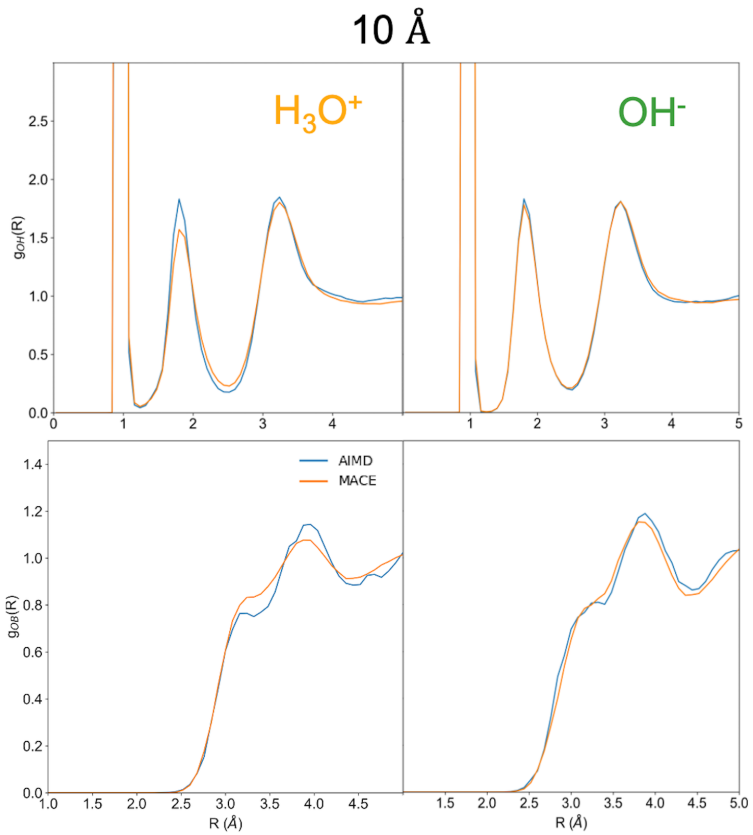

Figure S3: Radial distribution functions of O*H, O*B, of a hydronium and hydroxide ion oxygen atom using the trained MLIAP compared to a short 10 ps AIMD run for confined water at 10 $\mathring{A}$

2 Continued Data

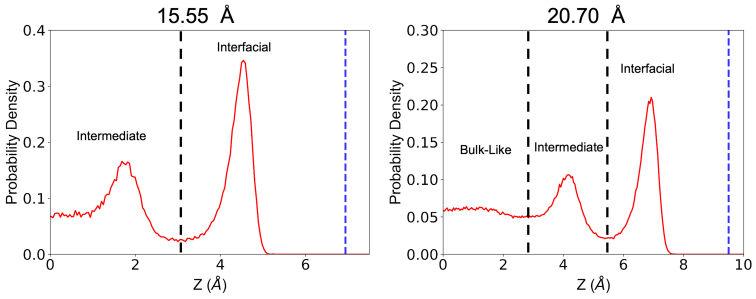

Figure S4: Probability density profile of oxygen atoms along the z-direction for two confinement distances, with water layers identified by the minima separating adjacent density regions.

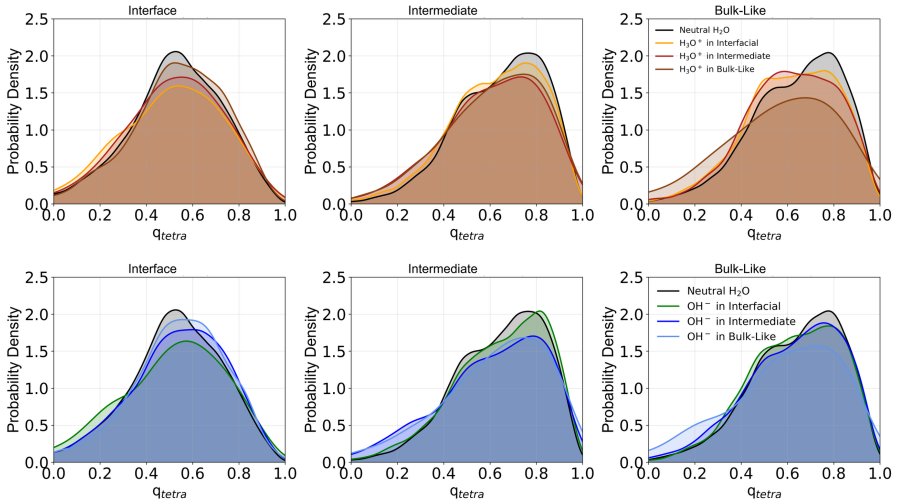

Figure S5: Probability density distributions of the tetrahedral order parameter for water molecules in the bulk-like region at a confinement distance of 20 as a function of the location of the water ion left) hydronium right) hydroxide. The plots compare three cases: (i) when the ion resides in the interfacial region, (ii) in the intermediate region, and (iii) in the bulk-like region. Each curve is shown relative to the probability density distribution of the tetrahedral order parameter for the interfacial, intermediate, and bulk-like water molecules in the neutral system. The regions are defined relative to the center of the slab being set as z=0.

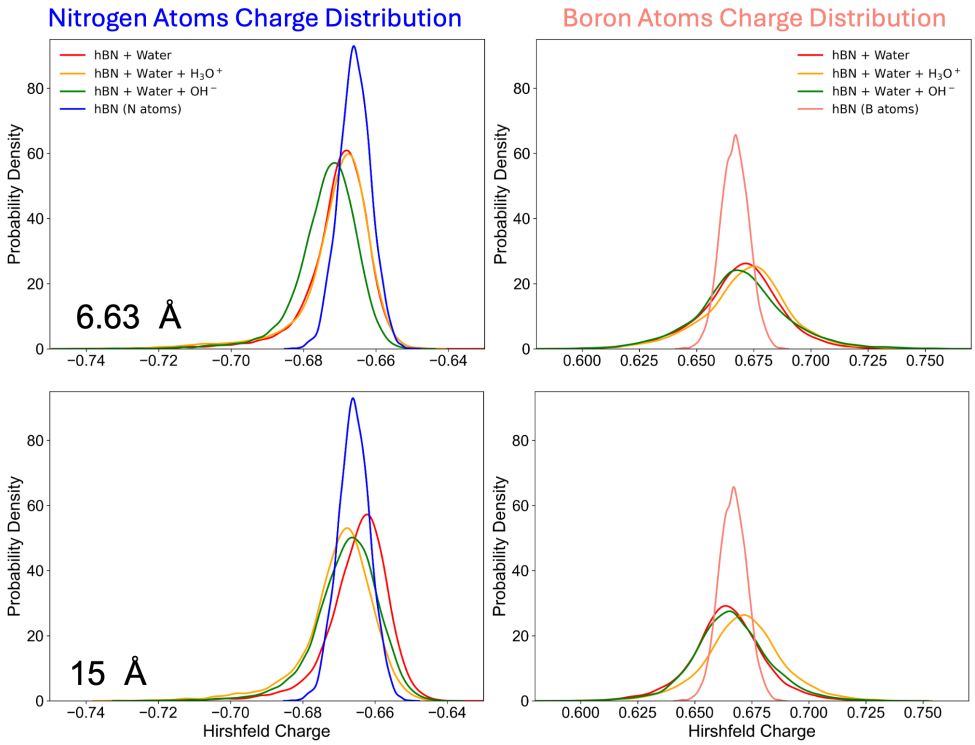

Figure S6: Probability distributions of the Hirshfeld charges on nitrogen and boron atoms for an hBN monolayer, confined neutral water between hBN sheets, and confined water containing either a hydronium or hydroxide ion.