

Supporting Information For:

Electric-Field Effects on Ionic Hydration: A Molecular Dynamics Study

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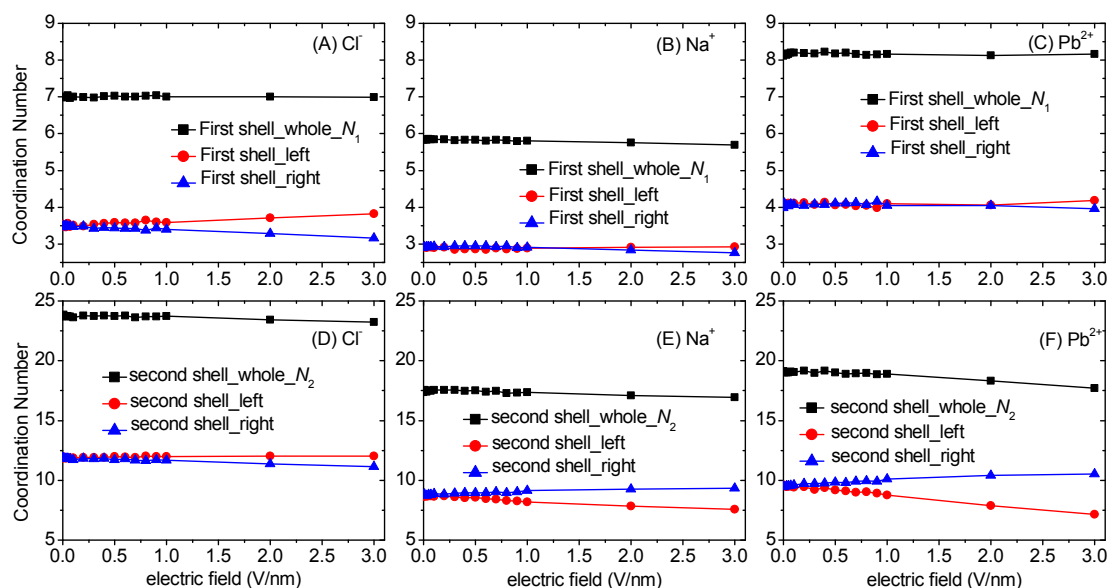


Figure S1. (A) Ion coordination number for the whole first hydration shell and the contributions from the left and right parts of the hydration shell along the field direction for (A) Cl^- , (B) Na^+ and (C) Pb^{2+} . For the second hydration shell (D) Cl^- , (E) Na^+ and (F) Pb^{2+} .

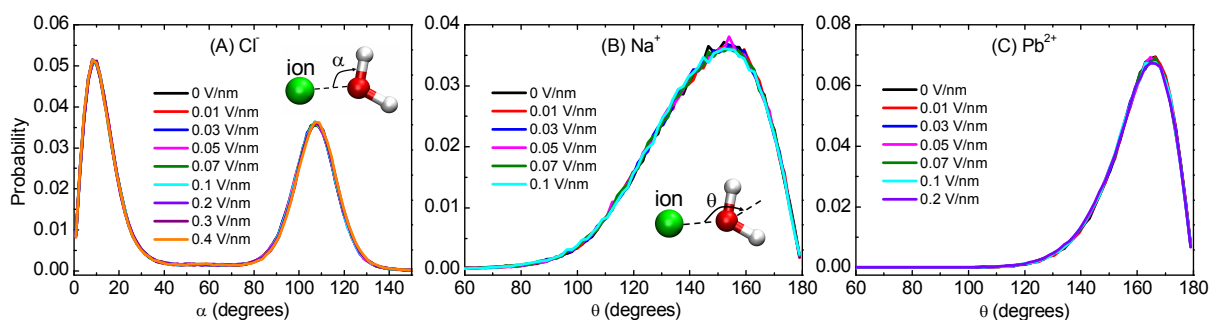


Figure S2. Probability distributions of the orientation angle α and θ of water molecules in the first hydration shell of (A) Cl^- , (B) Na^+ and (C) Pb^{2+} under weak fields (< 0.5 V/nm for Cl^- , < 0.2 V/nm for Na^+ and < 0.3 V/nm for Pb^{2+}). The insets show the definition of angle α and θ .

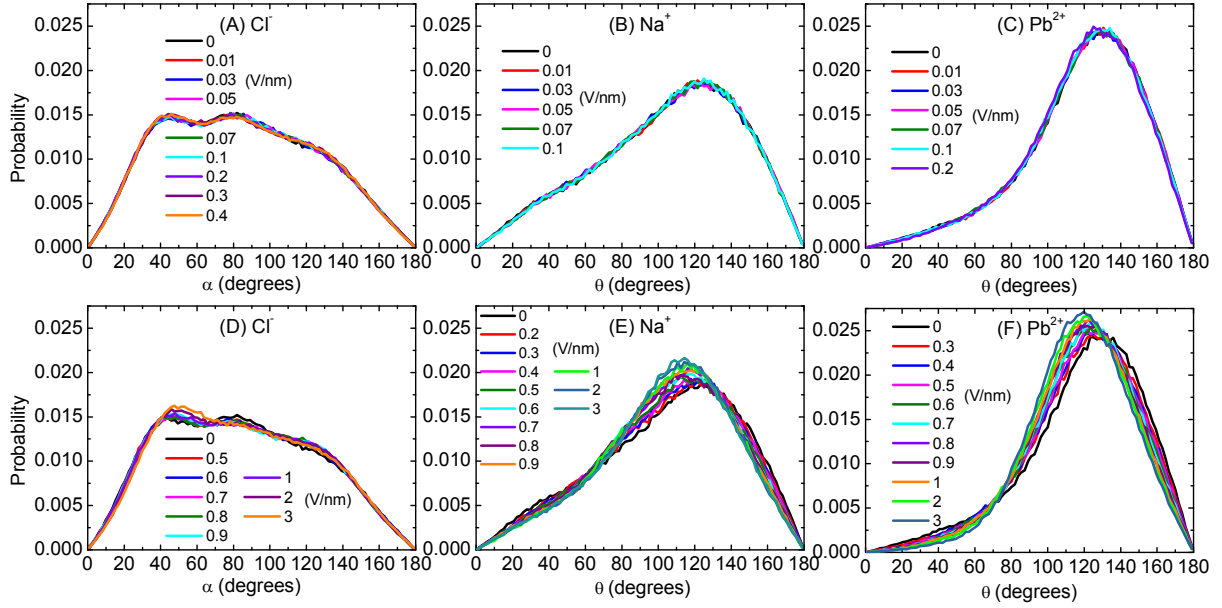


Figure S3. Probability distributions of the orientation angle α and θ of water molecules in the second hydration shell of (A) Cl^- , (B) Na^+ and (C) Pb^{2+} under weak fields (< 0.5 V/nm for Cl^- , < 0.2 V/nm for Na^+ and < 0.3 V/nm for Pb^{2+}), and (D) Cl^- , (E) Na^+ and (F) Pb^{2+} under strong fields.

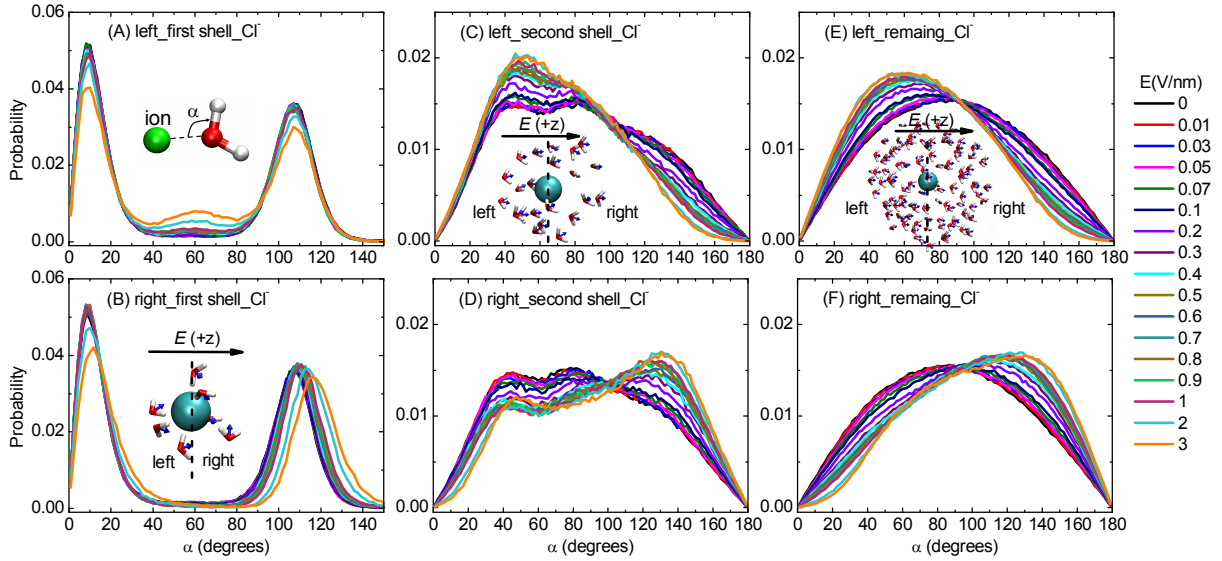


Figure S4. Probability distributions of the orientation angle α of water molecules in the left and right parts of (A,B) the first hydration shell, (C,D) second hydration shell and of (E,F) the remaining region of Cl^- along the field direction. The insets illustrate the dipole orientations of the water molecules in the first, second hydration shells and the remaining region of Cl^- under external fields.

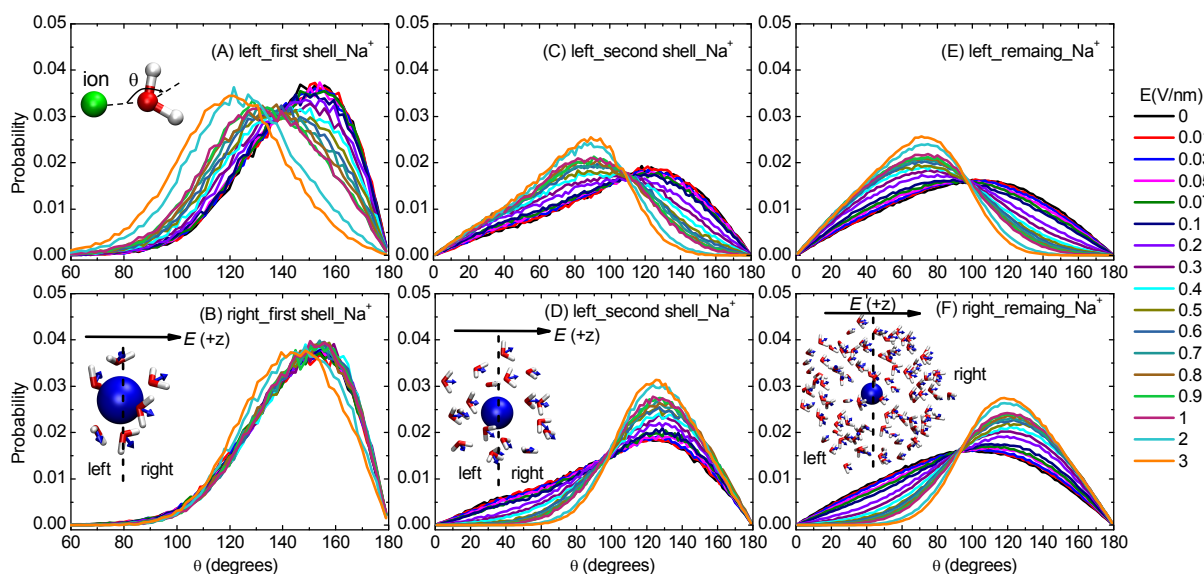


Figure S5. Probability distributions of the orientation angle θ of water molecules in the left and right parts of (A,B) the first hydration shell, (C,D) second hydration shell and of (E,F) the remaining region of Na^+ along the field direction. The insets illustrate the dipole orientations of the water molecules in the first, second hydration shells and the remaining region of Na^+ under external fields.

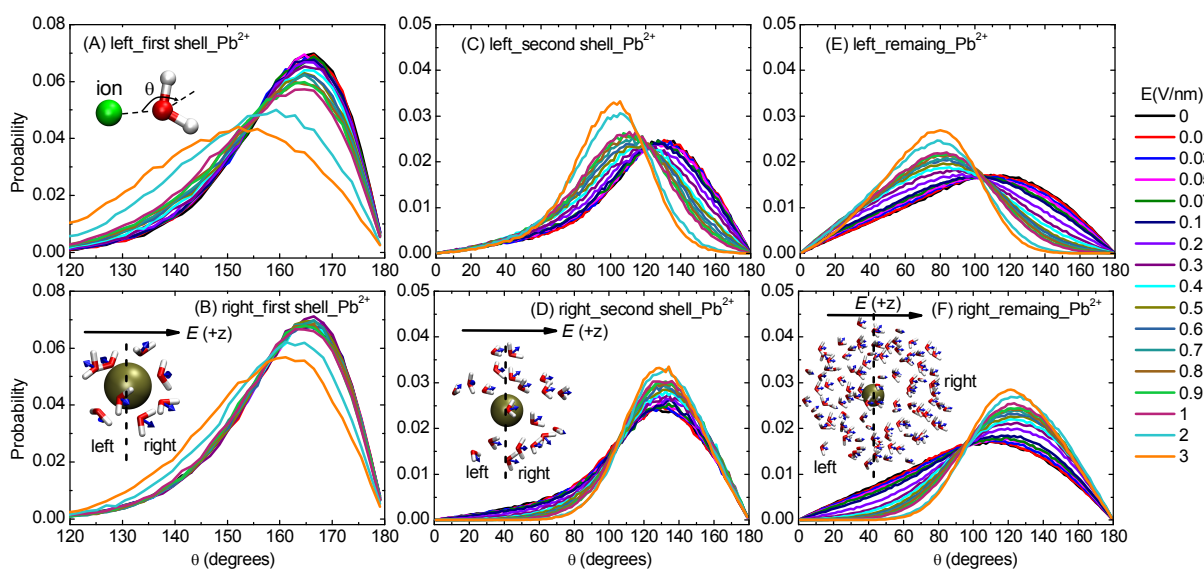


Figure S6. Probability distributions of the orientation angle θ of water molecules in the left and right parts of (A,B) the first hydration shell, (C,D) second hydration shell and of (E,F) the remaining region of Pb^{2+} along the field direction. The insets illustrate the dipole orientations of the water molecules in the first, second hydration shells and the remaining region of Pb^{2+} under external fields.

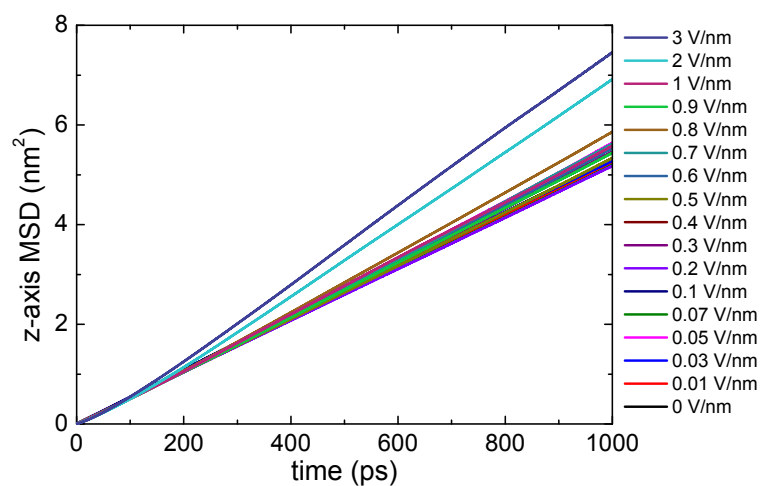


Figure S7. Mean square displacement (MSD) of oxygen atom in water molecules along the field direction (z-axis) under electric fields.