Supplementary Information (SI) for Physical Chemistry Chemical Physics.

Structure and dynamics of Li^{+}/Mg^{2+} confined in ZIF-8 under electric field from atomistic simulations

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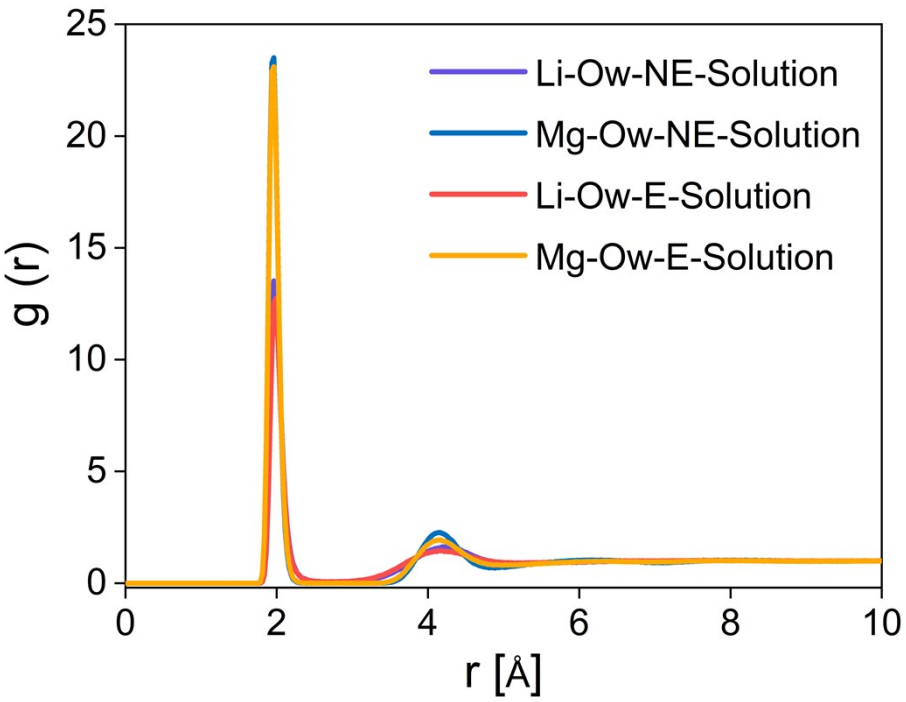
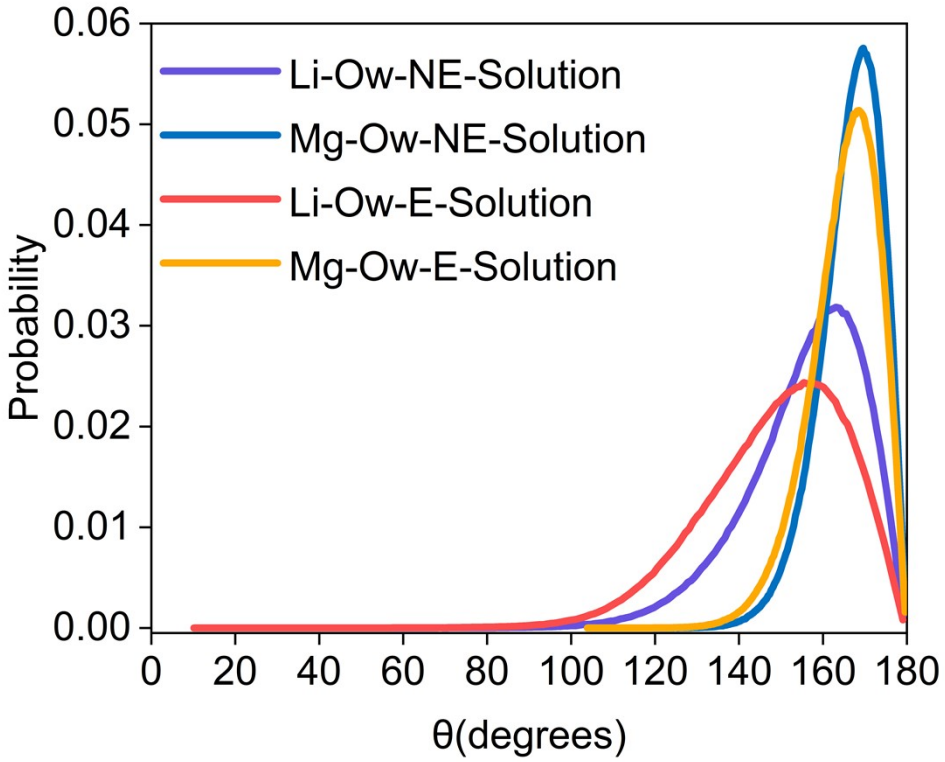
1. Ion−oxygen radial distribution functions g(r)



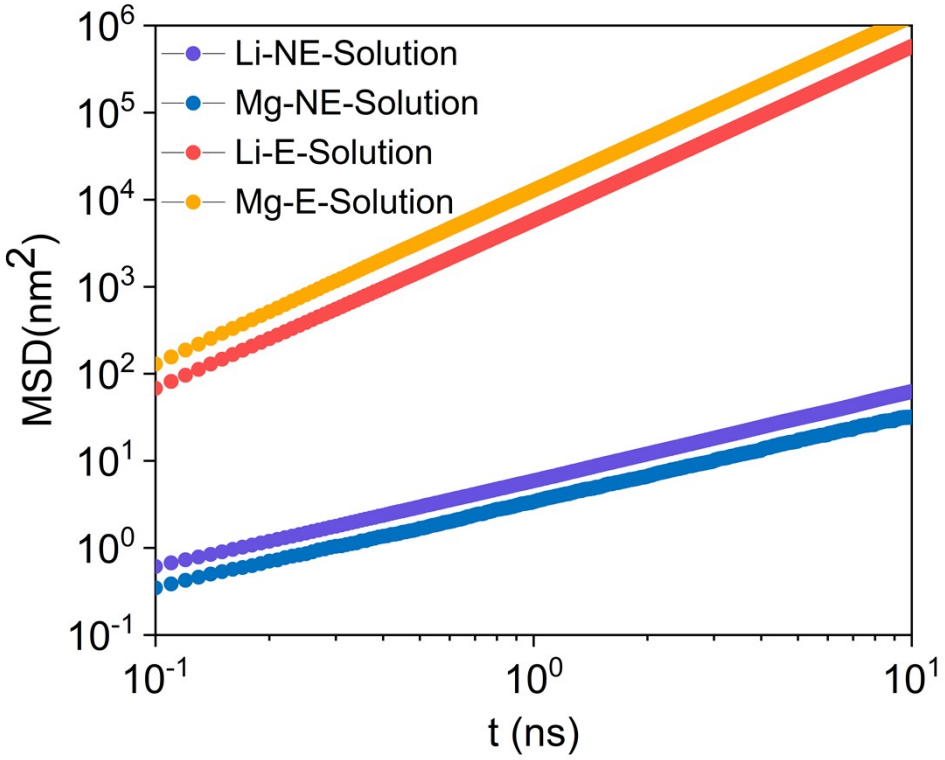
Figsure S1. Ion−water oxygen radial distribution functions g(r) of Li^+ and Mg^{2+} in aqueous solution. “E” and “NE” shown in legend indicate with and without external electric field, respectively.

2. Orientation angle distribution



Figsure S2. Probability distribution of water molecule orientation angle θ in the radius of the first hydrate layer in aqueous solution under different electric field conditions.

3. Mean square displacement



Figsure S3. Mean square displacement (MSD) of Li^{+}/Mg^{2+} in aqueous solution with different electric field conditions.