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Molecular Modeling of Structure, Diffusion, and Electrical Conductivity of Ionic Aqueous Solutions in Bulk and Confined within Nanoporous Media.

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This study is part of an extensive research program focused on the use of computational simulations to analyze the diffusion and electrical conductivity of ionic aqueous solutions in bulk and under nanoconfinement. We employed molecular dynamics (MD) simulations at OPLS-AA (Optimized Potentials for Liquid Simulations All Atom) + SPC/E (Extended Simple Point Charge) level to explore the structural and dynamic properties of sodium chloride (NaCl), potassium chloride (KCl), and lithium chloride (LiCl) in bulk aqueous solution. To quantify the effects of ion concentration and temperature, we calculated radial distribution functions (RDFs), coordination numbers, diffusion coefficients (D), and electrical conductivity for various concentrations (0.1, 0.5, 1.0, 2.0, 3.0, 4.0, and 5.0 M) and temperatures (20℃, 50℃, and 100℃). The radial distribution functions revealed that Li+ exhibits the lowest coordination number (3.6), indicating a compact and structured hydration shell due to its small size and high charge density. In contrast, Na+ (5.4) and K+ (6.6) show higher coordination numbers, suggesting more extended and diffuse hydration shells. These trends highlight that larger ions form less structured hydration shells with weaker ion-water interactions. It is worth noting that the coordination numbers obtained are in agreement with the experimental values reported in the literature. The analysis of diffusion coefficients reveals that heavier ions, such as K+ and Na+, under the same concentration and temperature conditions, exhibit faster diffusion within the fluid compared to Li+. Furthermore, as ion concentration increases, ion mobility decreases, while higher temperatures result in larger diffusion coefficients. To validate our MD model, we compared the calculated electrical conductivity values via the Nernst-Einstein equation with experimental measurements obtained using the open-ended coaxial reflection method. The results indicate that the MD simulations accurately reproduce the electrical conductivity of NaCl, KCl, and LiCl in aqueous solution at the ion concentrations studied in this work. To quantify the effect of nanoconfinement, we analyzed the structural and mobility properties of NaCl in solution confined within silica nanopores at various ion concentrations and pore sizes. The results show charge accumulation (double layer) near the surfaces of the solids. In addition, electrical conductivity increases as pore size increases. Finally, the presence of an external electric field results in increased ionic mobility and, consequently, higher electrical conductivity. These results highlight the use of MD simulations to provide a detailed molecular description of the structural properties and electrical mobility of ionic aqueous solutions in bulk and under nanoconfinement.

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References

Primary author: AMARO ESTRADA, Jorge Ivan (The University of Texas at Austin)

Co-authors: Prof. TORRES-VERDIN, Carlos (The University of Texas at Austin); Mr VILLARROEL SALVATIERRA, Julio C. (The University of Texas at Austin); Mr CRISAFULLI, Domenico Maria (The University of Texas at Austin)

Presenter: AMARO ESTRADA, Jorge Ivan (The University of Texas at Austin)

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