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Refined parameters for cations and anions in aqueous solution for atomistic force fields

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The assembly of metal surfaces, minerals, hydrogels, and biological systems can be significantly influenced by the presence of metal and nonmetal ions. Parameters for monovalent and divalent ions in molecular simulations have remained somewhat poorly rationalized and incomplete to date. We will discuss the development and validation of force field parameters for common mono- and di-valent cations (Li^+, Na^+, K^+, Rb^+, Cs^+, Be_2^+, Mg_2^+, Ca_2^+, Sr_2^+, Ba_2^+, Zn_2^+) as well as anions (F^-, Cl^-, Br^-, and I^-). The parameters reproduce experimental hydration energies, coordination numbers of water, and are consistent with trends in crystallographic size as well as approximate polarizability across the periodic table. They are compatible with the INTERAFCE force field, CHARMM, PCFF, and CVFF, including common water models such as SPC and TIP3P. Further validation also includes the densities of solid salts and their cleavage energies, providing consistent insight into solids and solid-liquid interfaces during dissolution and crystallization. The parameters can be used to explore morphologies and thermodynamic stability of inorganic and organic nanostructures.

Biography

Tariq Jamil is a PhD student in University of Colorado Boulder, USA. He has completed M. Eng., from NED University of Engineering and Technology. Currently, he is working under Dr. Hendrik Heinz on the topic Molecularly designed construction materials.

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