Innovating Workflows for the Development and Validation of Electrolyte Force Fields

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The accurate molecular simulation of ions is of high relevance for biological and chemical applications. Its complexity arises from the multiple interactions present between the ionic elements and their solvent. These interactions have to be properly considered and added to the set-up of a Molecular Dynamics (MD) simulation. Deviations in accuracy can lead to erroneous conclusions that can not be afforded in experimental applications. The effort to produce accurate ion models has resulted in multiple new force fields which were fitted to match specific target properties, but usually underestimate solubility values and cannot be universally applied.

OpenFF is among the list of models that have yet to make efforts towards developing accurate force fields for ions. This is specially relevant since OpenFF is highly focused on force fields for biomolecules, for which interactions with ions are inevitable. Consequently, the focus of our research has become to innovate workflows for the development and validation of electrolyte force fields that are convenient and effective for OpenFF developers to use in the near future. Our objectives to successfully achieve this include testing and benchmarking different water models, plus defining a set of optimization and validation parameters that ensure efficiency and accuracy for testing electrolyte force fields. The calculation of osmotic coefficients will be included in the validation parameters, since experimental data is widely available for salt solutions. These days, studies attempting to develop force fields using osmotic coefficients for the same purpose are scarce, due to the complexity of calculating the chemical potential of the water. The use of enhanced sampling methods allows us to overcome this challenge and to additionally obtain a large range of other thermodynamic properties that serve as optimization parameters, such as chemical potentials, osmotic pressure, hydration free energy, entropy and enthalpy.