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A review of molecular models for electrolyte solutions FREE

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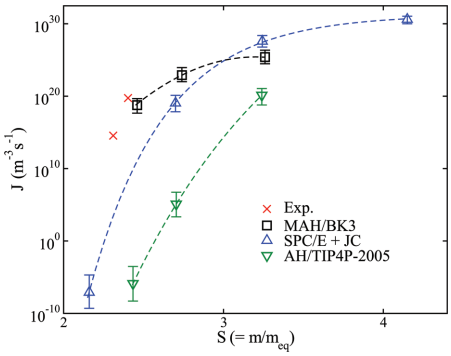
The perspective article finds that current models tend to fail in similar ways, implying the need to improve our current force fields for electrolytes in water.



There exists a need to develop accurate models for electrolyte solutions, which are important for biological and geophysical processes as well as technology. In particular, the "collective" properties of electrolyte solutions — such as activity coefficients and solubilities — are key for many applications. In the past, they have not been taken into account during the optimization of force field parameters because of high computational cost.

Athanassios Panagiotopoulos presents a review of methodological developments from the last several years that have enabled the efficient computation of these collective properties. He covers in detail recent molecular simulation studies and how their results compare to experimental data. In aggregating this information, Panagiotopoulos found that all the available practical models fail in similar ways, suggesting the need to include these properties when developing new potential models.

The article begins with a brief review of molecular models for water and simple ions in solution. It then discusses molecular simulation studies that calculate activity coefficients, solubilities, transport coefficients and nucleation rates. For each property, Panagiotopoulos summarizes current simulation methods, quantitative performance and transferability.

He concludes that, despite having advantages over phenomenological equations that can only describe a narrow set of properties, molecular simulations still have significant limitations. For instance, many models underpredict the solubility of salts in water at room temperature as well as elevated temperatures. This may be the reason why precipitation is often observed in simulations at very low salt concentrations. The review suggests ways to improve current models by including polarizability and charge transfer.

Additionally, because the majority of studies focus on the collective properties of NaCl, Panagiotopoulos recommends that the field examine whether the trends identified for NaCl carry over to other salts.

Source: "Simulations of activities, solubilities, transport properties, and nucleation rates for aqueous electrolyte solutions," by Athanassios Z. Panagiotopoulos, *Journal of Chemical Physics* (2020). The article can be accessed at http://doi.org/10.1063/5.0012102.