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Atomistic simulations of concentrated, multi-component liquids and biomolecular systems

Wednesday 25 September 2024 11:45 (45 minutes)

Molecular dynamics simulations with atomistic resolution are a standard tool to study liquids and biomolecular systems. Most often, force field (FF) limitations mean that simulations must be performed at low concentrations. I will discuss recent advances in FFs of ions and the insight they enabled into the molecular scale mechanisms leading to protein halophilicity, as well as the non-monotonic nature of solvation in multicomponent organic liquids revealed from simulations with high-quality FFs.

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