Bachelor Project

Biomolecular Dynamics
Stock Lab

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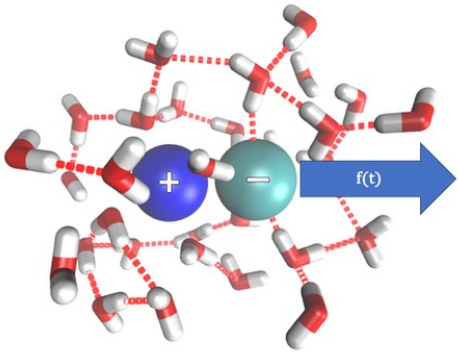
moldyn MolDynFR

Mimicking electronic degrees of freedom in MD simulations

Common Molecular Dynamics (MD) simulations use simplified point charge models to mimic the electrostatic potentials around a molecule. However, in highly charged environments, molecules may undergo changes in their electronic wave functions, that cannot be accounted for in such simplistic models. To avoid computationally expensive wave function calculations, polarizable force fields allow for an approximation of induced multipoles.

In this project, you will perform MD simulations to characterize the difference between a polarizable force field and a conventional fixed-charge force field for a pair of ions. Using various existing simulations of ion pairs embedded in water, you will furthermore calculate different experimental observables to assess which of the two approaches is in better agreement with real world data.



Useful information

Wolf, S., & Stock, G. (2018). Targeted Molecular Dynamics Calculations of Free Energy Profiles Using a Nonequilibrium Friction Correction. J. Chem.Theory Comput. 14, 6175–6182.

Talk to:

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