



ID de Contribution: 426

Type: Poster

Dissecting environmental effects on the dynamics of an ion in water through time-dependent friction

The motion of an ion in water is strongly affected by frictional effects from the surrounding solvent. Various theory have been put forward to characterize those effects and they feature a separability between mechanics part (short-ranged or Lennard-Jones forces) and dielectric part from the long range electrostatics. We study numerically the time-dependent friction from the water on monoatomic ions and explore the respective influence of those dielectric and hydrodynamics friction, identifying a strong anticorrelation between both part. This work opens the way to the building of a transferable friction for the coarse graining of the solvent.

Affiliation de l'auteur principal

Institut des Sciences du calcul et des données

Auteur principal: VROYLANDT, Hadrien (Institut des Sciences du Calcul et des données)

Orateur: VROYLANDT, Hadrien (Institut des Sciences du Calcul et des données)

Classification de Session: Session Poster 1: MC3, MC5, MC6, MC11, MC13, MC15, MC16, MC18, MC19, MC25, REDP, posters hors MC

Classification de thématique: MC13 Effets d'environnement et de solvation sur les processus moléculaires