

Cornell University Library

(Help | Advanced search)

Search or Article-id

arXiv.org > physics > arXiv:1107.4936

Physics > Chemical Physics

Atomistic simulations of electrolyte solutions and hydrogels with explicit solvent models

Jonathan Walter, Stephan Deublein, Steffen Reiser, Martin Horsch, Jadran Vrabec, Hans Hasse

(Submitted on 25 Jul 2011)

Two of the most challenging tasks in molecular simulation consist in capturing the properties of systems with long-range interactions (e.g. electrolyte solutions) as well as systems containing large molecules such as hydrogels. For the development and optimization of molecular force fields and models, a large number of simulation runs have to be evaluated to obtain the sensitivity of the target properties with respect to the model parameters. The present work discusses force field development for electrolytes regarding thermodynamic properties of their aqueous solutions. Furthermore, simulations are conducted for the volume transition of hydrogels in the presence of electrolytes. It is shown that the properties of these complex systems can be captured by molecular simulation.

Subjects: Chemical Physics (physics.chem-ph); Soft Condensed Matter (cond-mat.soft)

Cite as: arXiv:1107.4936 [physics.chem-ph] (or arXiv:1107.4936v1 [physics.chem-ph] for this version)

Submission history

From: Martin Horsch [view email] [v1] Mon, 25 Jul 2011 13:13:31 GMT (127kb)

Which authors of this paper are endorsers?

Link back to: arXiv, form interface, contact.

All papers 🚽 Go!
Download: • PDF • PostScript • Other formats
Current browse context: physics.chem-ph < prev next > new recent 1107
Change to browse by: cond-mat cond-mat.soft physics
References & Citations NASA ADS
Bookmark(what is this?)

