Physics > Chemical Physics

A transferable ab-initio based force field for aqueous ions

Sami Tazi, John J. Molina, Benjamin Rotenberg, Pierre Turq, Rodolphe Vuilleumier, Mathieu Salanne

(Submitted on 10 Apr 2012)

We present a new polarizable force field for aqueous ions (Li+, Na+, K+, Rb+, Cs+, Mg2+, Ca2+, Sr2+ and Cl-) derived from condensed phase ab-initio calculations. We use Maximally Localized Wannier Functions together with a generalized force and dipole-matching procedure to determine the whole set of parameters. Experimental data is then used only for validation purposes and a good agreement is obtained for structural, dynamic and thermodynamic properties. The same procedure applied to crystalline phases allows to parametrize the interaction between cations and the chloride anion. Finally, we illustrate the good transferability of the force field to other thermodynamic conditions by investigating concentrated solutions.

Comments:	31 pages, 8 figures
Subjects:	**Chemical Physics (physics.chem-ph)**; Statistical Mechanics (cond-mat.stat-mech)
Journal reference:	J. Chem. Phys. 136, 114507 (2012)
DOI:	10.1063/1.3692965
Cite as:	**arXiv:1204.2084 [physics.chem-ph]** (or **arXiv:1204.2084v1 [physics.chem-ph]** for this version)

Submission history

From: Mathieu Salanne [view email]
[v1] Tue, 10 Apr 2012 09:04:30 GMT (1373kb)

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