EGU22-32, updated on 26 Mar 2023
https://doi.org/10.5194/egusphere-egu22-32
EGU General Assembly 2022

Sodium/halides aqueous droplets in vacuo at the sub micron scale : size, temperature and concentration effects on their structural properties from simulations at the microscopic level.

Michel Masella[1], Vaérie Vallet[2], Florent Réal[2], and Céline Houriez[3]
[1]CEA Saclay, Institut Joliot, F-91191 Gif sur Yvette Cedex , France
[2]Laboratoire PhLAM, CNRS, UMR 8523, University of Lille, F-59000 Lille, France
[3]MINES ParisTech, PSL Research University, CTP - Centre Thermodynamique des Procédés, 35 rue Saint-Honoré, F-77300 Fontainebleau, France

We investigated sodium/halides (F, Cl, Br and I) aqueous droplets *in vacuo* at the microscopic level from molecular dynamics simulations at the 100 ns scale performed using a sophisticated polarizable all atom force field whose parameters are assigned only from high end quantum ab initio computations [1]. Long range electrostatic and polarizable forces are computed according to a Fast Multipole Method scheme devoted to polarizable force fields based on the induced dipole moment approach [2]. For Cl, Br and I we simulated 10k water droplets corresponding to 0.2, 0.6, 2.0 and 4.6 M salt concentrations and on a range of temperatures included between 260 and 320K. For F, we simulated 10k droplets corresponding to 0.2, 0.6, 0.8 and 1M salt concentrations. We also simulated a reduced set of salty droplets at 300K (in particular corresponding to NaCl salts) at the 100k (up to 100 ns) and at the 1M water molecules scale (up to 30 ns) [3]. We present here a detailed analysis of the structural properties of these droplets regarding ion spatial distributions, ion aggregates (size, composition, morphology, lifetime and distribution), water ordering (relative to pure water droplets) and droplet surface potentials. In the particular case of NaCl droplets, we also discuss droplet curvature effects on the latter properties from data corresponding to 10k, 100k and 1M systems.

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