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Atmospheric Chemistry and Physics Discussions

Interactive comment on "Molecular Dynamics Simulation of the Surface Tension of Aqueous Sodium Chloride: from Dilute to Highly Supersaturated Solutions and Molten Salt" *by* Xiaoxiang Wang et al.

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On p. 4, line 15, 3 references are given for the solubility of the SPC/E-compatible NaCl force field of Joung and Cheatham (JC):

The value is correctly given as 3.7 $\pm$ 0.2. However, the first reference (Paluch et al, 2010) provides a result (which is incorrect) for a different force field. The paper of Aragones et al (2012) gives an incorrect result for the JC force field. The correct value of 3.7 $\pm$ 0.2 is provided only in the final reference (Espinosa et al, 2016).

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Discussion paper

The first two references should be omitted, since the first is irrelevant and the second gives an incorrect result.

The history of the attempts to correctly calculate the aqueous solubility for the JC force field at 298.15K and 1 bar may be of interest.

The correct value of 3.7 ± 0.2 was first correctly calculated by my group:
author = Moučka, F. and Nezbeda, I. and Smith, W. R., title = Molecular Force Field Development for Aqueous Electrolytes: 1. Incorporating Appropriate Experimental Data and the Inadequacy of Simple Electrolyte Force Fields Based on Lennard–Jones and Point Charge Interactions with Lorentz–Berthelot Rules, journal = J. Chem. Theory Comput., volume = 9, number = 11, pages = 5076-5085, year = 2013

Our result was later corroborated by the Panagiotopoulos group:
author = Mester, Z. and Panagiotopoulos, A. Z., title = Mean ionic activity coefficients in aqueous NaCl solutions from molecular dynamics simulations, journal = J. Chem. Phys., volume = 142, number = 4, pages = 044507, year = 2015
and by Aragones et al. (2012) and Espinosa et al. (2016).

The history of the attempts to correctly calculate the quantity by molecular simulation are described in the following review article:
author = Nezbeda, I. and Moučka, F. and Smith, W. R., title = Recent progress in molecular simulation of aqueous electrolytes: force fields, chemical potentials and solubility, journal = Molec. Phys., volume = 114, number = 11, pages = 1665-1690, year = 2016

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