

Abstract Submitted
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Structural and electronic properties of NaCl dissolved in water¹

ALEX P. GAIDUK, Department of Chemistry, University of California, Davis, FRANCOIS GYGI, Department of Computer Science, University of California, Davis, GIULIA GALLI, Institute for Molecular Engineering, The University of Chicago — We carried out *ab initio* molecular dynamics simulations of a 1 M NaCl aqueous solution with the *Qbox* code, using the hybrid functional PBE0 and the bisection technique introduced in Ref. [1] to compute the Hartree–Fock exchange. We performed both NVT and NVE simulations. We found that the position of the Cl[−] and Na⁺ energy levels is considerably improved compared to the one obtained using the PBE functional, and that the anion highest occupied orbital [2] is unaffected by the presence of the sodium counterion. We also found that the average properties obtained in the NVE ensemble and those computed in the NVT ensemble with the Bussi–Donadio–Parrinello thermostat [3] are the same, within the statistical error bars of our simulations.

[1] F. Gygi and I. Duchemin, *J. Chem. Theory Comput.* **9**, 582 (2013).

[2] C. Zhang, T. Anh Pham, F. Gygi, and G. Galli, *J. Chem. Phys.* **138**, 181102 (2013).

[3] G. Bussi, D. Donadio, and M. Parrinello, *J. Chem. Phys.* **126**, 014101 (2007).

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