Abstract Submitted
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**Structural properties of simple aqueous solutions from ab initio simulations**[1] ALEX P. GAIDUK, Institute for Molecular Engineering, University of Chicago, FRANCOIS GYGI, Department of Computer Science, University of California, Davis, GIULIA GALLI, Institute for Molecular Engineering, University of Chicago — Although water and salt solutions have been studied for many decades, several aspects of their microscopic and electronic properties remain uncertain. One of the open questions is whether simple ions have long-range effects on the structure of liquid water. We performed extensive first-principles molecular dynamics simulations [1] of solutions of a simple salt (NaCl) and found that while $Na^+$ does not significantly change the structure of water beyond the first solvation shell, $Cl^-$ has a far-reaching hydrogen-bond-breaking effect. We present an analysis of the structural modifications in terms of molecular polarizabilities and dipole angular correlations. Our results are in agreement with the traditional classification of $Cl^-$ as a structure-breaker, but at variance with several theoretical and experimental studies which did not observe significant modifications of the structure of water outside the first solvation shell of ions [2]. We also present an analysis of the electronic properties of the solutions [3].

[1] *Qbox* code, http://eslab.ucdavis.edu/software/qbox/index.htm;
[2] Y. Marcus, *Chem. Rev.* **109**, 1346 (2009);
[3] A. P. Gaiduk, C. Zhang, F. Gygi, G. Galli, *Chem. Phys. Lett.* **604**, 89 (2014).

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