Abstract Submitted
for the MAR16 Meeting of
The American Physical Society

Photoemission spectra of aqueous solutions of salts from many-body perturbation theory[1] ALEX P. GAIDUK, JONATHAN H. SKONE, MARCO GOVONI, GIULIA GALLI, University of Chicago — The computational design of electrode materials for energy conversion and storage processes requires an accurate description of the energy levels of the electrolyte and of electrolyte/electrode interfaces. Conventional density-functional approximations are in general not well suited for this task as they yield inaccurate orbital energies. Many-body perturbation theory (MBPT) predicts vertical ionization potentials and energy gaps in better agreement with experiments, providing the possibility for an accurate description of the electronic properties of electrolytes. We coupled *ab initio* molecular dynamics [1] with MBPT calculations [2] to investigate the photoemission spectra of a 1 M aqueous solution of NaCl. For the first time we were able to determine the absolute positions of the spectra peaks, with excellent agreement with experiments for both the solute and solvent peak positions. The best results were obtained using wavefunctions obtained from dielectric-dependent [3] hybrid calculations as a starting point for MBPT.

[1] A. P. Gaiduk, C. Zhang, F. Gygi, G. Galli, *Chem. Phys. Lett.* 604, 89 (2014); [2] M. Govoni and G. Galli, *J. Chem. Theory Comput.* 11, 2680 (2015); [3] J. H. Skone, M. Govoni, G. Galli, *Phys. Rev. B* 89, 195112 (2014).

[1]Work supported by DOE BES DE-SC0008938. Computer time provided by the Argonne Leadership Computing Facility through the INCITE program.

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Date submitted: 27 Oct 2015 Electronic form version 1.4