Abstract Submitted
for the MAR14 Meeting of
The American Physical Society

Systematic investigation of the electronic and structural properties of chloride ion in aqueous solution by advanced density functional
ARINDAM BANKURA, CHARLES SWARTZ, MICHAEL L. KLEIN, XIFAN WU, Temple University — In a recent photoelectron spectroscopy (PES) experiment,[1] electron binding energies have been measured in aqueous chloride ion solutions. The position of the highest occupied molecular orbital (HOMO) of the chloride ion was found to be 1.25-1.50 eV above with respect to the valence band maximum (VBM) of water. Theoretically, we have computed the PES for the aqueous chloride ion solutions, in which the molecular solvation structures are generated from the *ab initio* molecular dynamics using gradient-corrected (PBE) and hybrid density functional (PBE0).[2] Using PBE level of theories we consistently found that HOMO level of the chloride ion on average below the VBM of the water. Whereas the HOMO of the anion was found above the VBM of water when the electronic structure calculations were carried out at the PBE0 level of theories. A substantial improvement in the result was found when the trajectory was generated using the corrections accounting for the effects of dispersion forces into the DFT-GGA scheme)[3]. and hybrid density functional.

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[2]X. Wu et al. Phys. Rev. B, **79**, 085102 (2009)
[3]A. Tkatchenko et al. Phys. Rev. Lett., **102**, 073005 (2009)

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Date submitted: 15 Nov 2013 Electronic form version 1.4