Abstract Submitted
for the MAR13 Meeting of
The American Physical Society

Vibrational spectroscopy of liquid water from first principles simulations: Raman Spectra[1] QUAN WAN, LEONARDO SPANU, Department of Chemistry, University of California, Davis, GIULIA GALLI, Department of Chemistry and Department of Physics, University of California, Davis, FRANCOIS GYGI, Department of Applied Science and Department of Computer Science, University of California, Davis — Raman spectroscopy is an important probe of the structural and vibrational properties of aqueous solutions and of water at interfaces. While many experimental data are available for various systems, no results of ab initio computations have yet been reported for the Raman spectra of liquid water or solutions. We computed the Raman spectrum of water at ambient conditions using first principles molecular dynamics simulations, coupled to the calculation of polarizability within density functional perturbation theory. We used semi-local functionals, 64 molecule cells and the Qbox code. Our results are in satisfactory agreement with experiment. We provided an interpretation of the spectral features oberved at low frequency and within the stretching band by defining a polarizability of water molecules in the fluid. Coupling the calculation of Raman and IR spectra is in progress: such coupling will open the way to interpret advanced vibrational spectroscopy measurements, e.g. Sum Frequency Generation spectroscopy.

[1]Work supported by DOE-CMSN DE-SC0005180

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Date submitted: 04 Nov 2012 Electronic form version 1.4