Abstract Submitted
for the MAR13 Meeting of
The American Physical Society

Large-Scale Hybrid-DFT First-Principles Molecular Dynamics[1]

WILLIAM DAWSON, FRANCOIS GYGI, University of California Davis — The recursive subspace bisection algorithm[1] is used to accelerate the computation of the Hartree-Fock exchange operator in hybrid-DFT, First-Principles Molecular Dynamics (FPMD) simulations. This approach provides a set of maximally localized orbitals in domains of variable size and allows for a reduction of the number of computed exchange integrals with controlled accuracy. It does not require a priori assumptions about the localization of orbitals in limited domains and can be used with both occupied and empty orbitals, thus enabling computations of the HOMO-LUMO gap during hybrid-DFT FPMD simulations. We discuss algorithmic improvements of the method and demonstrate its use in hybrid-DFT FPMD simulations of water, solvated ions, and a liquid-solid interface in which maximally localized orbitals show a wide range of localization properties. [1] F.Gygi, Phys. Rev. Lett. 102, 166406 (2009). [2] F. Gygi and I. Duchemin, JCTC (submitted). [3] http://eslab.ucdavis.edu/software/qbox/ .

[1]Supported by DOE BES DE-SC0008938

Francois Gygi
University of California Davis

Date submitted: 09 Nov 2012 Electronic form version 1.4