Abstract Submitted
for the MAR08 Meeting of
The American Physical Society

Order N Implementation of Exact Exchange XIFAN WU, Princeton University, ANNABELLA SELLONI, ROBERTO CAR — Exact (Hartree Fock) exchange is needed to overcome some of the limitations of local and semilocal approximations of density functional theory (DFT). Moreover exact exchange is a basic ingredient in modern approaches to compute excitation properties, like the GW and the OEP schemes. So far, however, computational cost has limited the use of exact exchange in plane wave calculations for extended systems. We show that this difficulty can be overcome by performing a unitary transformation from Bloch to Maximally Localized Wannier functions in combination with an efficient technique to compute real space Coulomb integrals. The resulting scheme scales linearly with system size and, when used in ab-initio molecular dynamics simulations, requires only a modest increase in computational cost compared to standard DFT implementations. We validate the scheme with representative applications.

Xifan Wu
Princeton University

Date submitted: 26 Nov 2007 Electronic form version 1.4