Abstract Submitted
for the MAR09 Meeting of
The American Physical Society

Functional minimization scheme for first-principles electronic structure calculations with bi-orthogonal interpolating wavelets WILLIAM GARBER, WEI KU, JAMES DAVENPORT, DMITRI VOLJA[1], Brookhaven National Laboratory — A new development of first-principles electronic method will be presented based on direct energy functional minimization and bi-orthogonal wavelet basis set. The employment of bi-orthogonal basis allows systematically controlled accuracy while benefiting from the compact support that allows O(N) algorithms. Furthermore, utilization of the interpolating nature of the wavelet, together with the effectiveness of multi-resolution of wavelet, enables very efficient calculation without compromising accuracy. By avoiding solving eigenvalue equation as in standard Kohn-Sham framework, the method is easily extended to parallel algorithms, and allows simple implementation of various non-local functionals. In case of crystals, our method gives directly solution as Wannier functions, further utilizing their sparseness. This new development is ideal for easy implementation and accurate systematic benchmarking of various modern functionals, and holds the potential to attack very large systems such as nano- materials.

[1]currently postdoc at MIT

William Garber
Brookhaven National Laboratory

Date submitted: 21 Nov 2008 Electronic form version 1.4