Abstract Submitted
for the MAR07 Meeting of
The American Physical Society

Adaptive multilevel Finite Element Method for Solving the Electronic Schrödinger Equation[1] ERIC BYLASKA, PNNL, MIKE HOLST, JOHN WEARE, UCSD — It is widely appreciated that to use computational methods for the design of materials encompassing a wide assortment of elements from the Periodic Table, highly efficient methods based as closely as possible on accurate quantum mechanics are needed. We have developed an O(N) ab initio molecular dynamics method based on an adaptive multilevel finite element first principles solver with an efficacious implementation of hybrid functionals . The matrix representations of the discrete Hamiltonian operator in the finite element basis are always sparse due to the local support nature of finite element basis functions. As a result, application of the Hamiltonian operator to a discrete function has complexity which is linear in the number of discretization points. This development also makes use of completely unstructured simplex meshes that have the advantage of giving resolution of the near singular features around atomic nuclei using minimal computational resources. Various aspects of the implementation and computational efficiencies will be discussed. This method has been applied to several systems including excitons in quartz, transition metal dimers, and aqueous complexes.

[1]support from the Advanced Scientific Computing Research program of the U.S. Department of Energy, Office of Science

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Date submitted: 28 Nov 2006 Electronic form version 1.4