Abstract Submitted
for the MAR10 Meeting of
The American Physical Society

**Linear-Scaling Density-Functional Theory with Tens of Thousands of Atoms: Expanding the Scope and Scale of Calculations with ONETEP** A.A. MOSTOFI, N.D.M. HINE, P.D. HAYNES, Imperial College London — ONETEP[1] is an *ab initio* electronic structure package for total energy calculations within density functional theory (DFT). It combines linear-scaling computational effort with plane-wave accuracy, through use of a systematically-convergable basis equivalent to plane-waves. We present recent progress improving the feasible scope and scale of of calculations with ONETEP. Efficient manipulation of sparse matrices (the Hamiltonian, overlap and density matrix expressed in a localized basis) is crucial to the performance of LS-DFT, and depends strongly on the suitability of the algorithms to a) the physics of the system, and b) efficient parallelization over thousands of processors. We present details of a scheme for matrix algebra employing hierarchical sparsity, optimized for calculations distributed over hundreds to thousands of parallel processors. Implementing this alongside new communications algorithms, we demonstrate a very considerable improvement in speed and parallel efficiency. We are therefore able to make calculations even for dense solid systems of tens of thousands of atoms routine, within comparably modest computational demands. This enables treatment of a range of new systems of technological interest, such as defect formation energies at grain boundaries in $Al_2O_3$.
[1] C-K. Skylaris *et al*, J.Chem. Phys. **122**, 084119 (2005).

Nicholas Hine
Imperial College London

Date submitted: 20 Nov 2009 Electronic form version 1.4