Abstract Submitted
for the MAR06 Meeting of
The American Physical Society

Atomic Forces and Geometry Optimisation with the ONETEP **Linear-Scaling DFT Method** ARASH MOSTOFI, Massachusetts Institute of Technology, USA, PETER HAYNES, Cavendish Laboratory, University of Cambridge, UK, CHRIS-KRITON SKYLARIS, Physical and Theoretical Chemistry Laboratory, University of Oxford, UK, MIKE PAYNE, Cavendish Laboratory, University of Cambridge, UK — ONETEP[1] (Order-N Electronic Total Energy Package), is a density functional method, based on plane-waves, whose computational cost scales only linearly with the number of atoms.
ONETEP uses a localised yet orthogonal basis of periodic cardinal sine (psinc) functions[2], also known as Dirichlet or Fourier Lagrange-mesh functions, which are formed from a discrete sum of plane-waves. The localised non-orthogonal generalised Wannier functions (NGWFs) which span the occupied subspace are represented in terms of these psinc functions and are optimised during the calculation.
This choice of basis and optimisation of the NGWFs results in smooth potential energy surfaces and enables the use of the Hellmann-Feynman theorem for the calculation of atomic forces. These have been implemented within a quasi-Newton geometry optimisation scheme and preliminary results are presented.

[1] *J. Chem. Phys.* **122**, 084119 (2005).
[2] *J. Chem. Phys.* **119**, 8842 (2003).

Arash Mostofi
Massachusetts Institute of Technology

Date submitted: 27 Nov 2005 Electronic form version 1.4