Abstract Submitted
for the MAR10 Meeting of
The American Physical Society

**A polarisable atomistic force-field for alumina parametrised using density functional theory** JOANNE SARSAM, MIKE FINNIS, PAUL TANGNEY, Department of Materials and Department of Physics, Imperial College London — We present an effective potential for bulk alumina ($Al_2O_3$), which has been parametrised by fitting the energies, forces, and stresses of a large database of reference configurations to those calculated with density functional theory (DFT). This approach, pioneered by Ercolessi and Adams [1], allows the construction of accurate force-fields without reference to experimental data, given a functional form which is capable of mimicking those electronic effects which dominate interatomic forces. Our functional form is simpler and less expensive than previous models of alumina parametrised by this technique. We compare our potential to those existing models [2], and to experimental and *ab initio* data on crystal structures and energies, elastic constants, phonon spectra, and thermal expansion. We demonstrate an overall accuracy that is close to that of DFT for these quantities. Some applications to the structure and diffusion of defects in corundum are discussed.

[1] F. Ercolessi and J. B. Adams. Europhys. Lett. **26**, 583 (1994). [2] S. Jahn, P. A. Madden and M. Wilson. Phys. Rev. B **74**(2), 024112 (2006).

Joanne Sarsam
Department of Materials and Department of Physics,
Imperial College London

Date submitted: 23 Nov 2009 Electronic form version 1.4