Application for a TSM-DTC funded PhD studentship

Please complete this form electronically
and submit to Lilian Wanjohi (l.wanjohi@imperial.ac.uk)
by Friday January 8, 2010

1st supervisor
Name: Dr Paul Tangney
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2nd supervisor
Name: Prof Norbert Klein
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3rd supervisors (optional)
Name: Prof Neil Alford and Prof Matthew Foulkes
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Please complete the following:

1. Project title Prediction of dielectric properties of Metal Oxides up to the Terahertz range.

2. Project abstract (≤ 200 words please and please add 1 or 2 key references)

Current microwave communications operate at around 2GHz and collision avoidance radar is around 70GHz. Future communications devices are predicted to use THz frequencies but very little is known about the properties of materials at THz frequencies.

Understanding the electrical properties of dielectrics for use in millimeter-wave and terahertz devices is vital for optimising performance. Using first-principle Density Functional Perturbation Theory, including anharmonic terms arising from phonon-phonon interactions, and effective Hamiltonian based molecular dynamics, this project will attempt to predict the complex permittivity of metal oxides starting with MgO, Al_2O_3 and TiO_2 progressing to perovskites from microwave up to terahertz frequencies. The Centre for Physical Electronics and Thin-Film Materials will soon have a powerful terahertz spectrometer, able to measure the complex permittivity from 30 GHz to 4.2 THz.   Using experimental data for bulk and thin-film dielectrics, theories will be developed to explain the observed dielectric behaviour.

3. What is the multi-scale nature of the project? (≤ 100 words please)
We will investigate dielectic response at a wide range of frequencies (timescales) – from very low frequency AC KHz to very high THz frequencies. We will examine the responses of bulk single crystals of mm size to thin films

nm thick. We will achieve this by parameterising effective Hamiltonians for large scale simulations of atomistic dynamics and high-frequency dielectric response from DFT and validate these models using Quantum Monte Carlo and DFT.

4. How do the expertises of the supervisors complement each other? (≤ 100 words please)

Klein and Alford – experimental and access to the new THz kit, Tangney and Foulkes on theory

5. Is there a self-contained 12-week MSc project that would usefully initiate this PhD project? (If the answer is no the project will not be offered as an MSc project)

Yes – Using existing highly accurate polarizable force-fields for MgO [6], TiO_2 [7], Al_2O_3, the dielectric response of perfect and defective crystals will be simulated and compared to the results of THz spectroscopy experiments performed by Professors Klein and Alford.

Suggested reading

[1] V. L. Gurevich and A. K. Tagantsev, Adv. Phys. **40**, 719 (1991).
[2] C. Herring, Phys. Rev. **95**, 954 (1954).
[3] M. Sparks, D. F. King, and D. L. Mills, Phys. Rev. B **26**, 6987 (1981).
[4] R. Stolen and L. Dransfeld, Phys. Rev. **139**, 4A (1965).
[5] . P. Tangney and S. Scandolo, "An ab initio parametrized interatomic force-field for silica" J. Chem. Phys. **117** 8898 (2002)
[6] P. Tangney and S. Scandolo, "A many-body interatomic potential for ionic systems: application to MgO," J. Chem. Phys. 119, 9673 (2003).
[7] X. J. Han, L. Bergqvist, P. H. Dederichs, *et al.* "A polarizable interatomic force field for TiO_2 parameterized using density functional theory", submitted to Phys. Rev. B; arXiv:0911.5311.
[8] S. Baroni, S. de Gironcoli, A. Dal Corso, *et al.* "Phonons and related crystal properties from density-functional perturbation theory", Rev. Mod. Phys. **73**, 515 (2001).
[9] W. M. C. Foulkes, L. Mitas, R. J. Needs, *et al.* "Quantum Monte Carlo simulations of solids" Rev. Mod. Phys. **73**, 33, (2001).