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
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3rd supervisor (optional)
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Please complete the following:

1. Project title

Multiscale Theory and Simulation of Nanoscale Ferroelectric Materials

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

Ferroelectric materials have diverse applications, from fast random access memory to tunable microwave devices, electrocaloric refrigeration, thermoelectric power generation and gate oxides in transistors. The drive toward miniaturisation of ferroelectric materials raises intriguing questions

regarding the nanoscopic nature of the ferroelectric effect as the ferroelectric domain size becomes only a few unit cells in extent. On the mesoscopic scale, the pattern of ferroelectric domains exhibits a non-trivial dependence on sample shape and size[1].

This project aims to develop a coarse-grained model to describe the static and dynamic properties of nanoscopic domains at the mesoscopic scale. The theory will be built up from the ab initio level with electronic structure calculations based on density-functional theory on interfaces between ferroelectric domains. This information will be coupled to semi-empirical atomistic potentials that will be used to perform molecular dynamics simulations and to probe the dielectric response to electric fields on length scales of 10s of nanometers. These atomistic models will inform the development of mesoscopic Ginzburg-Landau-like models that will be used to understand the dynamics of domains as a function of sample size and shape. It is hoped that this theoretical effort will be supported by an experimental programme of research, including in situ electron microscopy of domain dynamics.

3. What is the multi-scale nature of the project? (≤ 100 words please)

Ab initio density-functional theory calculations; atomistic molecular dynamics; development of coarse-grained mesoscopic models for domain dynamics.

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

Dr Tangney is an expert on density-functional theory and the development of classical atomistic potentials[2,3]. Dr Mostofi is an expert on large-scale density-functional calculations[4,5]. Prof McComb is a world-leader in electron microscopy and the theory of domain dynamics.

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. Scanning transmission electron microscopy images of ferroelectric nanodots using a high-angle annular dark-field (HAADF) detector show patterns that are consistent with theoretically-predicted vortex polarisation domain structures [1]. However, it is unknown why/whether polarisation domains are observable with HAADF imaging. We will attempt to resolve this mystery and to correctly interpret the HAADF images. Using Rutherford scattering theory, and classical electromagnetism to map the electromagnetic force on an electron as it passes through a sample containing patterned polarization domains, you will model the HAADF image that should be observed and compare directly to experimental results.

[1] A. Schilling, D. Byrne, G. Catalan, *et al.* "Domains in Ferroelectric Nanodots", Nano Lett. **9**, 3359 (2009).
[2] P. Tangney and S. Scandolo, "An *ab initio* parametrized interatomic force-field for silica" J. Chem. Phys. **117** 8898 (2002).
[3] P. Tangney and S. Scandolo, "A many-body interatomic potential for ionic systems: application to MgO," J. Chem. Phys. 119, 9673 (2003).
[4] N. D. M. Hine, P. D. Haynes, A. A. Mostofi, C.-K. Skylaris and M. C. Payne, "Linear-scaling density-functional theory with tens of thousands of atoms: Expanding the scope and scale of calculations with ONETEP", Comput. Phys. Commun. **180**, 1041 (2009).

[5] C.-K. Skylaris, P. D. Haynes, A. A. Mostofi and M. C. Payne, “Introducing ONETEP: Linear-scaling density functional simulations on parallel computers”
J. Chem. Phys. **122**, 084119 (2005).