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: Professor Adrian Sutton
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2nd supervisor
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3rd supervisor (optional)
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4th supervisor (optional)
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Please complete the following:

1. Project title A multi-scale model for deformation of polymers

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

Polymers and especially polymer composites are becoming increasingly important in structural applications e.g. in aerospace, and as functional materials in plastic electronics. They are also used as membranes for filtration, and Professor Livingston's group in Chemical Engineering is world-leading in the design and development of these membranes. In all these applications there is a need to develop a coarse-grained model of how polymer chains rearrange themselves during deformation processes. This project will develop a coarse-

grained representation of polymer chains as flexible elastic wires, which interact with each other and with particles. The interactions will be calculated using state-of-the-art linear scaling DFT methods (ONETEP) with van der Waals interactions. The bending modulus of the polymer chains will also be calculated using DFT methods. The algorithm MILC-SHAKE, which was recently developed by Aimee Bailey, a PhD student at Imperial working in collaboration with the University of Amsterdam [1,2], will then be used to construct the coarse-grained representation of the polymer, building in the interactions calculated by DFT methods. A particular application will be to understand through simulation the chemical and physical factors that determine the porosity of polymer films grown in Professor Livingston's group.

[1] "Efficient constraint dynamics using MILC SHAKE", A G Bailey, C P Lowe and A P Sutton, J. Comp. Phys., **227**, 8949-8959 (2008).
[2] "REVLD: A coarse grained model for polymers", A G Bailey, C P Lowe and A P Sutton, Comp. Phys. Commun. **180**, 594-599 (2009).

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

There are three length scales involved. At the atomic scale first principles methods will be used to determine the strength of chemical bonds, short-range repulsive interactions, and van der Waals interactions. At the second, larger length scale the atomistic detail is stripped away and attention is focused on the deformation processes of the polymer chains represented as elastic wires, subject to the constraints imposed by the short and long range interactions computed at the electronic structure level. At the third length scale, the structure of the polymer film will be described using the simulations of the polymers as elastic wires.

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

Dr Mostofi is an expert in DFT methods and their use in ONETEP to carry out first-principles simulations. Professor Sutton and coworkers have applied the elastic wire representation of single polymer chains to describe their dynamics in solution. Professor Livingston is a world-leader in the design and manufacture of polymer films with controlled porosities.

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, it would involve the writing of a code to model the disentanglement of an entangled interacting elastic wire using MILC-SHAKE to represent the chain as a sequence of short inextensible straight segments.