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: Robin Grimes
CID (IC only): Institution, Department, Address: Imperial College, Department of Materials.
Email:r.grimes@imperial.ac.uk
Phone:0207 594 6730

2nd supervisor
Name: Mark Wenman
CID (IC only): 600593
Institution, Department, Address: Imperial College, Department of Materials.
Email:m.wenman@imperial.ac.uk
Phone:0207 594 6763

3rd supervisor (Industrial collaborators)
Name: Kurt Atkinson
CID (IC only):
Institution, Department: Fuel Performance Group, British Energy,
Email: kurt.atkinson@british-energy.com
Phone: 01452 656352

4th supervisor
Name: Blas Uberuaga
CID (IC only):
Institution, Department: MST-8, Los Alamos National Laboratory, New Mexico, USA
Email: blas@lanl.gov
Phone:

Please complete the following:

1. Project title

Radiation damage mediated processes in nuclear fuels

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

Although radiation damage in UO_2 has been modelled extensively, relatively little has been done on MOX fuels, inert matrix fuels (e.g. Zr/U/Pu O_2 solid solutions) or on advanced fuels (e.g. uranium silicide and thoria based systems). This project would involve the use of ab initio methods to predict atomic scale structures, molecular dynamics to predict dynamic damage processes at the atomic scale on ps time scales and accelerated dynamics techniques (in collaboration with Blas Uberuaga at Los Alamos) to predict the evolution of

processes on much longer time scales. The distribution of fission products would be a particular emphasis of the project. Results from these simulations will be used to develop phenomenological models for fuel behaviour, which will be incorporated into existing industrial fuel performance codes (in collaboration with the ENIGMA British Energy fuel performance team and the TRANURANUS team at ITU).

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

The project involves multi-time scale modelling approaches. Normal ab initio methods can only reach time scales of picoseconds. However, work using these methods can then be used to create molecular dynamics simulations. Time accelerated dynamics (TAD) can then be used to investigate migration of fission product species which do not diffuse on picosecond timescales in the material.

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

Prof Robin Grimes is the head of the Centre for Nuclear Engineering at Imperial College and has 20 years experience of modelling nuclear fuel materials, especially ceramics and radiation damage, at the atomic scale. He has strong links to the fuel modelling community both here and abroad.

Dr Wenman has considerable experience of modelling of materials for nuclear applications especially nuclear fuels and regularly meets the fuel team at British Energy to feed his research into their fuel performance modelling.

Dr Kurt Atkinson is a senior member of the fuel performance Group at British Energy, who develop and maintain the industry standard fuel performance code ENIGMA. This code is also used by the UK National Nuclear Laboratory and Westinghouse.

Dr Uberuaga will be a strong collaborator to this project. Dr Uberuaga is an expert in radiation damage of nuclear materials and specialises in the use of TAD for studying diffusion of atomic species created by irradiation damage such as vacancies and interstitials.

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. The student would begin by carrying out a project using ab initio and molecular dynamics methods for studying defects and fission products in thoria nuclear fuels. This will introduce the student to using ab inito to study…..