

Radiation damage is known to lead to materials failure and thus is of critical importance to the lifetime and safety within nuclear reactors. Its detrimental effects can be prevented by appropriate advanced nanomaterials tailoring, inherent to which are composition and structure modelling. Due to the multi-scale nature of the problem, experts in the fields of materials simulation via *ab initio*, molecular dynamics and continuum modelling are building up ever-growing teams to contribute to the characterization and improvement of such highly demanding materials. It is in this context where a

THREE-YEAR POSTDOCTORAL RESEARCH FELLOW APPOINTMENT AT THE UNIVERSITY OF OVIEDO (SPAIN)

for a talented and motivated individual is offered.

Expected starting date: From October the 15th, 2011 (could also start at a later convened date).

The University of Oviedo was established in 1608. It is a public institution, with more than 1500 researchers and 250 research groups, devoted to higher education teaching and research that fosters the social, economic and cultural development of the local community through the generation and diffusion of knowledge. Today, it has become the main research centre of the Principado de Asturias, a Spanish autonomous region with a population of over one million inhabitants located in the north-west of Spain. Nanotechnology related research is very active at UNIOVI, with more than 100 researchers and the cooperation in the recently created Research Center on Nanomaterials and Nanotechnology (CINN). Both fabrication, characterization and modelling areas are present, the latter through the scientific and technological modelling computing cluster and the new supercomputing center which is being established this year.

The appointed researcher will work in a young but enthusiastic environment, based in Oviedo. The researchers involved in this particular work package participate in several HPC (High Performance Computing) initiatives through the RES (Spanish Supercomputing Network) and HPC Europe. Close collaboration with the University of Burgos, IMDEA-Materials (Madrid) and the Nuclear Fusion Institute (DENIM, Madrid) is envisaged. Permanent collaborations with international institutions, as Los Alamos National Laboratory (USA), Lawrence Livermore National Laboratory (LLNL), Georgia Tech Lorraine University (Metz, France), University of Tartu (Estonia), University of Uppsala (Sweden), or Paul Scherrer Institute (PSI, Switzerland), have been established.

Lines of research:

- ✓ Multiscale modelling of advanced nano-structured materials for engineering applications under extreme environments.

- ✓ Advanced materials in next generation fission nuclear reactors and the new inertial confinement and magnetic fusion initiatives. ESFRI – HiPER EU project and DEMO international collaboration.
- ✓ Integration in the very attractive scientific developments of ever-growing international research community involved in fusion materials technology.

The research activity will concern atomistic mechanisms and materials properties at interfaces of interest. The Post Doctoral fellow will help develop atomistic scale interfacial models relevant to our multiscale modelling program by means of *ab initio* calculations using commercially widespread packages, such as Wien2k and VASP, already available within our group. Other first principles simulation packages (Abinit, SIESTA, QuantumESPRESSO,...) could possibly be used at some stage to perform specific computations.

Previous experience with density-functional calculations based on plane waves and pseudopotentials is requested. Experience in *ab initio* simulations on surfaces and a basic knowledge on the foundations of density functional theory are highly recommended. Expertise in installation and running of computer codes in parallel environments is required. The applicant should be able to work with Linux, have at least a basic scripting knowledge, as well as be acquainted with Fortran and C programming languages. Expert handling of visualization tools is a plus.

Since the results obtained from the first principle calculations will be used as an input for molecular dynamics and lattice kinetic Monte Carlo codes in order to analyse defect evolution at experimentally relevant time frames, familiarity in the use of such techniques would be advantageous.

The Post Doctoral fellow will be working in a highly collaborative environment in close synergy with experimentalists from other institutions. Therefore, research performed at large facilities, such as an X-ray synchrotron or neutron sources, will be highly appreciated. Both theoretical and experimental background in fields related to nuclear materials science would also be of great interest.

Finally, the applicant should be able to fluently communicate in English. Spanish basic knowledge would be helpful.

The interested candidates should submit (in PDF-format) their (1) curriculum vitae, (2) publication list, and (3) one reprint of representative previous research. The interested candidate should also express his/her motivation in a covering letter, including the prospected date of availability, and arrange confidential letters of recommendation to be sent to the address below. Only complete applications will be processed. The selection process will continue until a suitable candidate occupies this opening.

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