



## POST-DOCTORAL POSITION AT CEA

### Atomistic modeling of the impact of magnetism on thermodynamic and diffusion properties of Fe-Cr-C alloys

CEA Saclay – DEN/DANS/DMN/SRMP

A 24-month post-doctoral position is available, from October 2018, at the physical metallurgy laboratory of CEA Saclay (SRMP: Service de Recherches de Métallurgie Physique).

The Fe-Cr and Fe-Cr-C systems are model alloys of ferritic/martensitic steels, which are proposed as structural materials for future fission and fusion nuclear reactors. Depending on their temperature, composition and microstructure, Fe-Cr-C alloys can be paramagnetic or ferromagnetic. The magnetic state is known to be an essential physical parameter of the phase equilibria and the properties of point defects, such as the formation and migration energies of vacancies and self-interstitials. Therefore it affects a broad range of thermal and transport properties involving diffusion, segregation and precipitation occurring in alloys at high temperatures and under irradiation.

The objective of the project is to develop an effective interaction model, based on first principle calculations, providing with a precise description of the effect of the atomic magnetic configuration on the point defect properties (vacancies, self-interstitials and carbon atoms) in Fe-Cr alloys. This model will be implemented in atomistic kinetic Monte Carlo simulations taking explicitly into account the evolution of the magnetic and chemical degrees of freedom, to study the effect of the ferro/paramagnetic transition on the diffusion coefficients of Fe, Cr and C atoms or the kinetics of Cr segregation and precipitation.

The project will be within the framework of the European program M4F (Multiscale modeling for fusion and fission materials), in collaboration with several groups and especially with the Culham Centre for Fusion Energy.

The salary will be around 3100€ per month.

We are looking for a well-motivated post-doctoral researcher, with strong skills in atomistic modelling of materials and a solid background in statistical physics. A good knowledge on programming is also required.

Interested candidates will submit by email an application letter, a detailed CV including a list of publications and two reference names.

#### Contact persons

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