Direction de la recherche fondamentale (DRF) Institut Rayonnement Matière (IRAMIS) Service de Physique de l'Etat Condensé – SPEC



Postdoctoral research position at CEA-Saclay, France

Tight-binding spin-lattice dynamics in binary Fe alloys

A 12-month postdoctoral position (with possible 12-month extension) is open in the laboratory of Physics of the Condensed State (SPEC: Service de Physique de l'état condensé) in CEA-Saclay.

Subject description:

Magnetic properties of materials are intimately linked to their structural properties. Iron is a characteristic example since its equilibrium crystallographic structure (bcc) is stabilized by the magnetism. More generally in iron-based alloys such as Fe-Cr the magneto-elastic coupling has a drastic influence on their physical properties (stability, kinetics etc). To model these alloys in realistic conditions it is thus necessary to describe the magnetism and the structure at the same level.

In this project we propose to develop and implement a magnetic tight-binding molecular dynamics code in which the time evolution of the structural and magnetic degrees of freedom are treated on the same footing. In this approach the electronic and magnetic structure of the material will be described by an efficient non-collinear magnetic TB model that has already been validated for iron and its alloys. The spin dynamics will be described by the Landau-Lifshitz-Gilbert equation of motion of the localized magnetic moments.

The code will be applied to the modeling in realistic conditions of of Iron and Iron-based alloys (in particular FeCr) which play an important role as structural materials for numerous technological applications.

The successful candidate is expected to implement a magnetic tight-binding molecular dynamics code.

The salary is around 3100€ per month. The position is available before December 2017.

Skill requirements:

Applicants should hold a Ph.D degree in Solid State Physics or Materials Science or a closely related discipline, with expertise/experience in simulations of magnetic systems and good skills in programming (e.g. FORTRAN, C, etc.). An experience in tight binding modelling is considered as a plus. Applicants should provide a **CV**, a **list of publications** and two **reference letters**.

Contacts:

| Cyrille Barreteau | Chu-Chun Fu | Pascal Thibaudeau |
|----------------------------|----------------------------|--------------------------|
| CEA Saclay | CEA Saclay | CEA Le Ripault |
| DRF/IRAMIS/SPEC | DEN/DANS/DMN/SRMP | BP16, F-37260 |
| 91191 Gif-sur-Yvette Cedex | 91191 Gif-sur-Yvette Cedex | Monts, |
| France | France | France |
| Tel: +33 1 69 08 38 56 | Tel: +33 1 69 08 29 32 | Tél: 02 47 34 46 56 |
| cyrille.barreteau@cea.fr | chuchun.fu@cea.fr | pascal.thibaudeau@cea.fr |