



## Post-doctoral position

### Thermodynamic properties of iron-based alloys: the key role of magnetism

12 months post-doctoral position is available, starting January 2020, at the “Laboratoire d’Etude des Microstructures” (<http://lem.onera.cnrs.fr/>) in Paris (France).

Iron-based alloys (such as steel) are one of the most important structural materials. Their versatility stems from a large number of alloying elements that are employed and from different microstructures that are generated in sophisticated heat treatments and other processing steps. The development of new Iron-based alloys with specific properties is thereby still largely empirical. A key factor that makes a rational design approach harder than for other materials is magnetism. Indeed, magnetism is a quantum property of materials and its impact on thermodynamic, kinetic or mechanical properties is far from obvious.

The aim of this postdoctoral position is to gain a better insight into the role of magnetism on the thermodynamic properties of iron-based alloys. This work will be carried out at the atomic scale using a tight-binding formalism perfectly adapted to this very particular physics. Finite temperature mechanisms will be studied via Monte Carlo simulations to handle systems containing up to a few hundred or even a thousand atoms. In practice, bulk systems such as pure iron and FeCo alloy will be investigated to characterize the importance of magnetism on thermodynamic properties. This project will be developed in close collaboration with French and German partners.

Applicants should have a Ph.D. (condensed matter physics, materials science or physical chemistry) and experience in electronic structure calculations and computer simulation techniques. Knowledge of tight-binding models would be a real advantage. Qualified candidates should send their curriculum vitae and a description of their research experience and interests to:

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