

# EXMONAN

AMSTERDAM (The Netherlands) from 25-29 June, 2018

---

## **Coupling Electronic Structure to Atomistic Simulations for Modelling Metallic Magnetic Materials**

Christine Goyhenex

Institut de Physique et Chimie des Matériaux de Strasbourg, Université de Strasbourg,  
CNRS UMR 7504, 23 rue du Lœss, BP 43, F-67034 Strasbourg, Cedex 2, France

Alloys and nanoalloys receive much attention because of their numerous potential applications in various fields like metallurgy, catalysis, magnetism, optics and health [1]. One main scientific challenge is to model their structure and properties as accurately as possible in order to participate to the design of new materials with targeted properties. Computer materials design is indeed a flourishing area with the development of simulations platforms, easily accessible for users. Nevertheless, if the proposed simulations tools are more and more sophisticated, some progress can still be expected for energy models (or interaction potentials) on which the simulations are founded. Such models would indeed deserve some improvements by getting closer to the electronic structure. In particular, taking magnetism into account in energy expressions, would be an important step forward for a better description of segregation and ordering phenomena when interested in magnetic materials and alloys including nanoalloys [2, 3, 4]. Based on recent works on the environment dependence of magnetic moment within the tight-binding approximation [5, 6], a methodology to generalize the tight-binding expression of the energy to account for magnetism will be presented. The work will be illustrated in the particular case of pure Co materials and CoPt alloys, going from perfect bulk to alloy surfaces and nanoalloys.

### References:

- [1] R. Ferrando, J. Jellinek, and R. L. Johnston *Chem. Rev.* 108 (2008) 845; R. Ferrando, *Structure and Properties of Nanoalloys*, Elsevier, 2016, vol. 10.
- [2] S. Karoui, H. Amara, B. Legrand and F. Ducastelle, *J. Phys.: Condens. Matter* 25 (2013) 056005.
- [3] C. Goyhenex, L. Zosiak, R. Kozubski, G. Tréglia, *J. Phys. Cond. Matter*, 27 (2015) 455503.
- [4] M. Sansa, F. Ribeiro, A. Dhouib, G. Tréglia, *J. Phys. Cond. Matter*, 28 (2016), 064003.
- [5] C. Goyhenex, G. Tréglia, B. Legrand, *Surf. Sci.*, 646 (2016) 261.
- [6] M Sansa, A Dhouib, F Ribeiro, B Legrand, G Tréglia and C Goyhenex, *Modelling Simul. Mater. Sci. Eng.*, 25 (2017) 084004.