Design of metastable phases with novel electronic properties

Andrea Gauzzi[1,⋆]

[1] *Sorbonne Université-IMPMC, CNRS, IRD, MNHN, 4, place Jussieu, 75005 Paris.*

Abstract. Extreme thermodynamic conditions, such as high pressures in the GPa range and above, offer the unique opportunity of stabilizing metastable phases with unusual structural and electronic properties [1,2]. For instance, high pressure increases the width of the electronic bands, thus favoring metallic properties, and tends to stabilize structures with high coordination numbers (or high-density). In previous years, these general guidelines have led to the discovery of several novel phases with remarkable properties, such as superconductivity at the surprisingly high temperature of 203 K in H_2S [3], or ultrahard phases [4]. The challenge is an effective search of novel phases with the desired electronic and functional properties. In order to face this challenge, a powerful research strategy is the combination of *ab initio* calculations of the total energy and of the electronic structure with *in situ* probes, such as x-ray diffraction. In this lecture, I shall provide an introduction to the topic by illustrating selected examples of novel metastable phases that have been successfully synthesized under high pressure, such as transition metal oxides with multiferroic properties and transition metal sulfides exhibiting heavy-fermion behavior. I shall also provide an overview on some recent advances in the theoretical and experimental methods used to effectively search for novel phases, with emphasis on *in situ* synchrotron x-ray diffraction.

References

[1] J. V. Badding, Ann. Rev. Mater. Sci. **28**, 631 (1998).

[2] P. F. McMillan, Nature Materials **1**, 19 (2002).

[3] A.P. Drozdov, M.I. Eremets, I.A. Troyan, V. Ksenofontov, S.I. Shylin, Nature **525**, 14964 (2015).

[4] Q. Gu, G. Krauss, W. Steurer, Advanced Materials **20**, 3620 (2008).

⋆e-mail: andrea.gauzzi@upmc.fr