



Subject:

Two-year post doctoral position in condensed matter computational physics/chemistry: application to the simulation of NMR spectroscopy

Message:

A two-year position is offered in the framework of a cooperative project funded by the French National Agency for Research (ANR). The three following partners are involved in this project called LoCharATMO (for Local characterization of alkali-transition metal oxides and polyanionic compounds): M. Ménétrier and D. Carlier at the “Institut de Chimie de la Matière Condensée de Bordeaux” (<http://www.icmcb.u-bordeaux1.fr/>), F. Boucher at the “Institut des Matériaux Jean Rouxel de Nantes” (<http://www.cnrs-imn.fr/>) and L. Le Pollès at “Sciences Chimiques de Rennes” (<http://scienceschimiques.univ-rennes1.fr/>). The position is immediately available and will be mostly based in Nantes.

The candidate should have a solid background in DFT calculations for periodic systems with experience in the treatment of correlated electrons (GGA + U, hybrid functionals, etc.) and a good culture of materials science. Communication skills are also required in this cooperative project.

CV, letter of motivation as well as the contact details of at least 2 references should be directed to F. Boucher : Florent.Boucher@cnrs-imn.fr.

Description of the research:

Alkali-transition metal oxides and polyanionic compounds exhibit very complex and unique properties such as redox activity associated to alkali diffusion for Li battery materials and peculiar electronic properties suitable for thermo-electricity generation. A particularly relevant method for approaching the local structure of these compounds is **NMR spectroscopy**. It is indeed sensitive to the atomic, electronic and magnetic local environment of a large number of nuclei, many of which are quite common in the materials of interest (Li, Na, Co, P, O if enrichment in the ^{17}O isotope is possible, possibly F etc.). NMR is also sensitive to dynamic effects in a rather wide range of time scales (from tens of MHz to Hz). However, the richness of the information carried by NMR is often obscured by the complexity of the interactions that govern the signal in such complex materials, and the lack of understanding of some of these interactions, notably the so-called hyperfine ones, exerted by delocalized or single electrons onto the nuclei probed by NMR. **Improvement of the understanding of such interactions is therefore a key to the full exploitation of NMR in these systems.**

Concerning the interpretation of the paramagnetic NMR contact shift, a modelling strategy,¹ based on the VASP code, was previously used. It estimates the electron spin density transferred from the transition metal to the nucleus site probed by NMR in order to assist assignment of NMR signals and understand the mechanisms of this transfer. The aim of the present project is to improve this strategy by the calculation of the hyperfine field using an all electrons method and/or PAW implementations. The correlation with NMR experiments will be done by the knowledge and interpretation of magnetic susceptibilities.

The other aspect of the project is making use of the developments of by J. H. Kristensen and I. Farnan in 2001 for modelling of anisotropic line shape changes due to movement,² typically to Na NMR signals in layered cobaltates. This will be done in close collaboration with I. Farnan (<http://www.esc.cam.ac.uk/people/academic-staff/ian-farnan>).

¹ *Understanding the NMR shifts in paramagnetic transition metal oxides using density functional theory calculations.* Carlier D., Menetrier M., Grey C. P., Delmas C. and Ceder G. *Phys. Rev. B* **67**, 174103 (1-14) (2003)

² *Disorder and dynamics in pollucite from ^{133}Cs and ^{27}Al NMR.* Ashbrook S. E., Whittle K. R., Le Pollès L., Farnan I., *Journal of the American Ceramic Society* **88**, 1575-1583 (2005)

