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Biography

Marie-Bernadette Lepetit has completed her PhD at the Université Paul Sabatier in Toulouse France on the ab-initio treatment of the electronic correlation. She has obtained a research position in the Laboratoire the Physique Quantique, CNRS in 1988 where she stayed until 2004. In 2004, she moved to the CRISMAT in Caen as a CNRS Director of research where she initiated a theory group. In 2012, she then moved to Grenoble where she joined the Institut Néel and Institut Laue Langevin where she headed the theory group until recently. From 2008 to 2015, she headed the French National Research Group (GdR) on strongly correlated materials gathering more than 450 researchers. Recently she is heading the committee program for high performance computing in chemistry and is member of the French National Committee for Scientific Research (electronic structure in condensed matter section). She is a Theoretician, specialist of the ab-initio treatment of electronic and magnetic excitation in strongly correlated materials. She works at the interface of solid state physics and quantum chemistry and aims at solving the structure-properties relationships in strongly correlated systems.

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THE ROLE OF THE RARE-EARTH ON THE MANETO-ELECTRIC COUPLING: THE RMN2O5 FAMILY

Magneto-electric, multiferroic material have attracted a lot of attention in the last decade due to their ability to control their polarization or dielectric constant using a magnetic field, or to control their magnetic order using an electric field. Among these materials the RMn2O5 family is a prototypal system as in some of its members the coupling between the electric and magnetic properties is among the largest, as was first shown by Hur et al. In the RMn2O5 family the magneto-electric coupling originates in the release of the magnetic frustration between the manganese ions. However, according to the nature of the rare-earth, the coupling can either be large as in the Tb compoud or nill as in the Sm one. Similarly, the polarization can take quite different values. For instance, the GdMn2O5 compound exhibits an extremely large polarization of about 3600μC/m2. In this talk we will try to present a comprehensive model explaining the role of the rare earth both on the existence of a magneto-electric coupling and the magnetic order, as well as on the polarization amplitude.

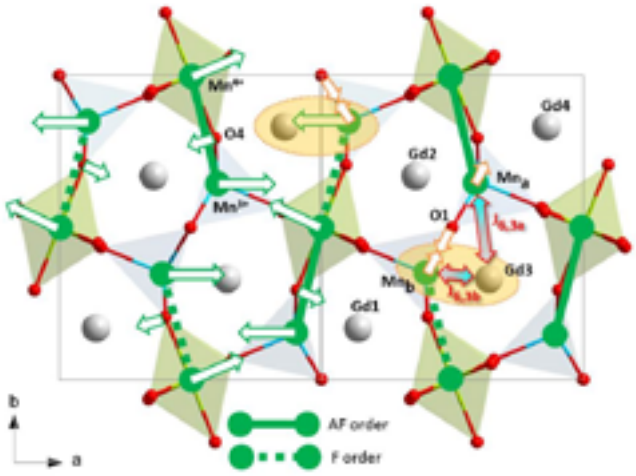

Figure.1: Atomic displacements associated with the release the magnetic frustration at the origin of the polarization.

Recent Publications

1. G Yahia, F Damay, S Chattopadhyay, V Balédent, W Peng, E Elkaim, M

Whitaker, M Greenblatt (2017). Recognition of exchange striction as the origin of magnetoelectric coupling in multiferroics. Phys. Rev B95: 184112.

2. G Yahia, F Damay, S Chattopadhyay, V Balédent, W Peng, S W Kim, M Greenblatt, M B Lepetit and P Foury-Leylekian (2018). Experimental evidence for the microscopic mechanism of the unusual spin-induced electric polarization in GdMn2O5. Phys. Rev B 97: 085128.
3. W Peng, V Balédent, S Chattopadhyay, MB Lepetit, G Yahia, C Colin, M J Gooch, C R Pasquier, P Auban-Senzier, M Greenblatt, P Foury-Leylekian (2017). Toward pressure induced multiferrocity in PrMn2O5. Phys. Rev. B 96, 054418.
4. V Balédent, S Chattopadhyay, P Fertey, M B Lepetit, M Greenblatt, B Wanklyn, F O Saouma, J I Jang et P Foury-Leylekian (2015). Evidence for room temperature electric polarization in RMn2O5 multiferroics. Phys. Rev. Letters 114, 117601.
5. Marie-Bernadette Lepetit (2016). How to compute the magneto-electric tensor from ab-initio calculations. Theor. Chem. Acc 1: 135.

Note: