Proposal of PhD thesis for 2024

« Modeling of properties of type II - multiferroic materials by numerical simulations »

Multiferroic (MF) materials are materials that possess spontaneous magnetic order (i.e. local magnetization) and electric polarization (i.e. in the absence of magnetic field and electric field) below a temperature called the transition temperature. These materials have significant potential for technological applications in the field of very high-density information storage and spin electronics. In the latter case, the challenge consists of controlling/manipulating the local magnetization of the material using an electric field, which would allow very significant energy savings. However, we are still far from the ideal MF material for which it would be possible to control the local magnetization with a weak electric field at room temperature and which would have a large electric polarization that could easily be "reversed". This project therefore concerns the study, by numerical simulations, of existing MF materials with the aim of better understanding and confirming/disproving/completing the experimental results as well as the study of new potentially MF materials (doped materials for example). This work will be based on realistic modeling based on *ab initio* calculations using density functional theory and on Monte Carlo simulations. The properties studied will be magnetic order at low temperatures, phase transitions, manipulation of local magnetization using an electric field and manipulation of electric polarization using a magnetic field. This work should make it possible to highlight conditions for improving the properties of MF materials, in particular increasing their transition temperature for future applications at room temperature.

Keywords : multiferroics, antiferromagnetism, magnetic frustration, helical magnetic order, magneto-electric coupling, phase transitions, Monte Carlo simulations, ab initio calculations.

Skills required : the candidate should have good skills in magnetism in solids, in statistical thermodynamic and should be attracted to numerical simulations.

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