First-principles study of RMn_2O_5 magnetoelectric multiferroics

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Recently, compounds in the RMn_2O_5 series, with orthorhombic crystal structure, have been the subject of intense research for their potential in the design of new single phase magnetoelectrics [1,2]. RMn_2O_5 belong to the so-called type-II class of multiferroics, with the ferromagnetic and ferroelectric modes generating each other. Complex magnetic structures, a relatively strong coupling between magnetization and polarization, various dielectric and magnetic phase transitions versus temperature, as well as small values of the polarization and critical temperatures have been reported [3,4]. In order to exploit the properties of these materials for applications, theoretical research accompanying experimental investigations has focused on the development of models to explain the complex dielectric and magnetic phase diagrams, the mechanism of magnetoelectric coupling, as well as the orbital magnetism and orbital magnetoelectric response in finite electric fields [5-7].
In this contribution we present results of first principles calculations within the density functional theory on bulk RMn_2O_5 compounds, with R standing for a rare earth element, Y and Bi, aiming at: i) the determination of the ground state magnetic structure and polarization; ii) the response to an applied electric or magnetic field, in the linear-response regime; iii) the exploration of the energy surface in these systems. We also discuss the role of oxygen antiferromagnetic spin polarization in the magnetoelectric coupling, as derived from the present calculations, and in relationship with recently reported neutron scattering results [8].

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