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DFT simulations applied to multiferroic materials

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Now-a-days, superficial process is very important for chemical reactions, optical, electrical and magnetic properties. Ab-initio simulations are very specific for molecular structure, electronic density, spin, charge and others quantum information. Surface models have been developed to clarify and understand the electronic nature and properties; the Density Functional Theory (DFT) is one of more applied quantum descriptions used in surface science in molecular structure. Multiferroic materials have been researched because of its structure to represent a material with two or more properties. One special case is the electro-magnetic coupling in R3 and R3c structures as bulk superficial dimensions can contribute significantly to develop transdutors and spintronic devices. Our experience in simulating multiferroic materials is presented in analysis of electronic structure directed to electronic levels and spin location from magnetic cations. However, a particular phenomenon is described in literature as the possibility to localize spin density in Ti atom became it a Ti^{3+} specie, which is very important to understand the intermetallic connection in materials with two cations, more specifically one magnetic cation and other non-magnetic cation. Such spin localization indicates band-gap reduction and spin channels from magnetic induction in a non-magnetic cation.

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