THE STUDY OF SOME ELECTRICAL AND MAGNETIC PROPERTIES FOR THE BULK AND SURFACE OF Fe_3O_4 AND OTHER BINARY COMPOUNDS BY *AB INITIO* METHODS

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Abstract

Development of computing power has allowed more close parallel between theoretical aspects of science of materials and experimental data, as well as their direct interpretation on the basis of the proposed models. *Ab initio* methods constitute some of the tools of cuanto-chemical calculations for approaching of the crystalline structures.[1] This work is a first step in an attempt to justify the superparamagnetic behavior of particles of Fe3O4 micrometer-sized [2,3]. We also propose the study of some electronic and energetic properties and structure parameters both in volume and surface for ZnS and CdS, both belonging to the crystalline phase of the P 63mc space group. To this end we used the Hartree-Fock hamiltonian with GTF-Pople sets of base function for optimization of structures, as well as Kohn-Sham hamiltonian with different exchange-correlation functionals for DFT calculations. Given the large number of electrons involved in the primitive cell we was forced to use the effective core pseudopotentials (ECP) to model the inner layers electrons.

References

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