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NATIONAL UNIVERSITY OF ENGINEERING, FACULTY OF SCIENCES, LIMA, PERU

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Electronic Structure of Bismuth Ferrite in Different Crystal Phases

Shigueru Nagata
National University of Engineering
Email: snagatat@uni.pe

Summary

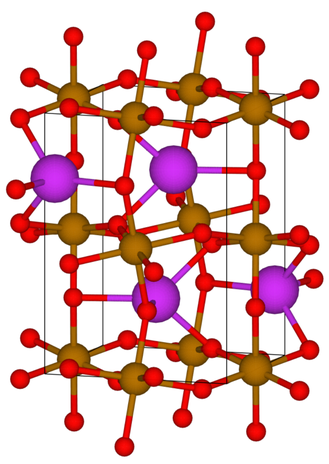
The electronic structure of different phases of Bismuth Ferrite were calculated by using density functional theory. Our results have shown that in case of R3c and Pnma Bismuth Ferrite has G-antiferromagnetic ordering. In all calculated structures, Bismuth Ferrite is a semiconductor with the band gap: 2.0 eV for R3c and 0.8 eV for Pnma.

Introduction

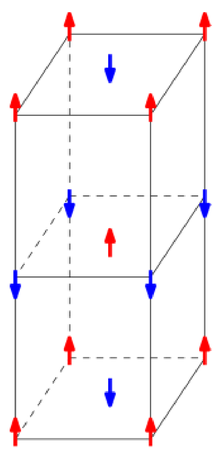
Bismuth Ferrite ($BiFeO_3$) is the room-temperature multiferroic compound which have attracted an increasing interest due to its potential applications for magnetoelectric devices[1]. In this work we focus on the electronic structure of aforementioned phases of $BiFeO_3$ calculated withim density functional theory approach.

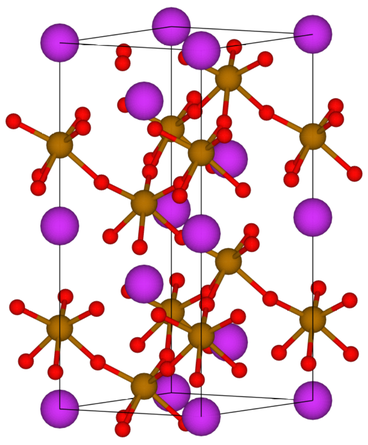
Method of calculation

The calculations were done by using the plane waves method (PW) as implementend in Open-source Package for Research in Electronic Structure, Simulation and Optimization (QUANTUM ESPRESSO) version 6.3. The Perdew-Burke-Ernzerhof (PBE) were used for exchange-correlation potential. The Brillouin zone integrations were performed by using 4x4x4 Γ-centered k-point grid. A kinetic energy cutoff of 517 eV and a total energy convergence thresold of 10^{-6} eV were used. All the structures were fully relaxed and the obtained lattice constants and atomic coordinates were used for futher



Pnma



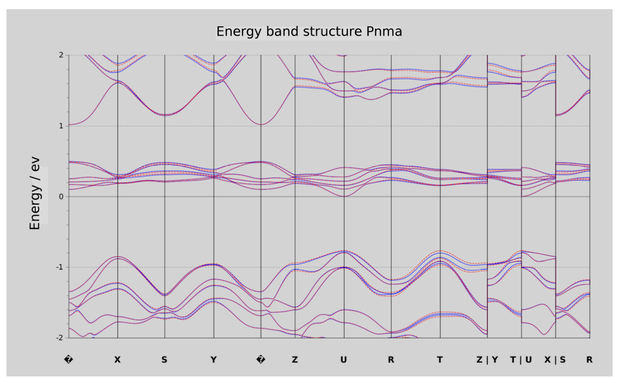


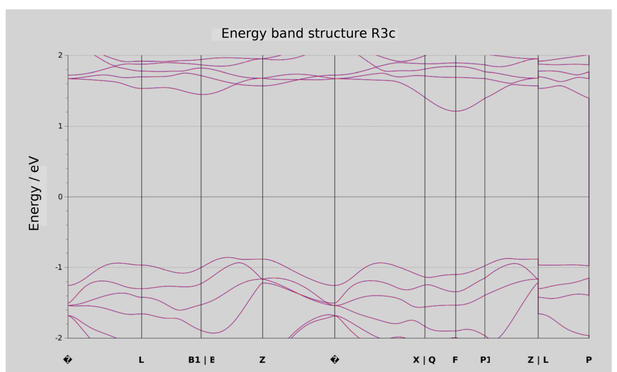
R3c

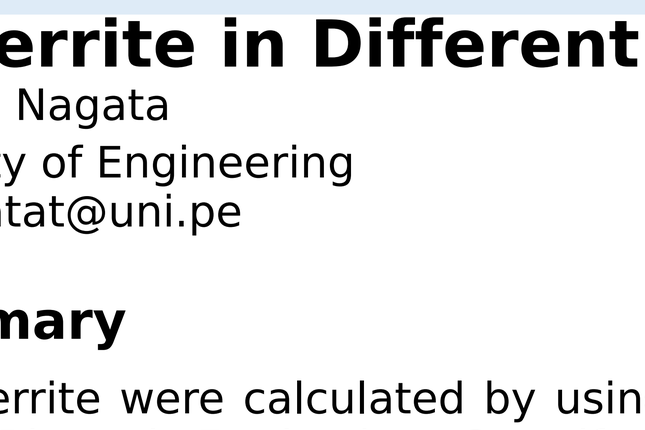
Fase	a (Å)	b (Å)	c (Å)
r3c	7.893	7.893	7.893
pnma	7.830	7.830	7.770

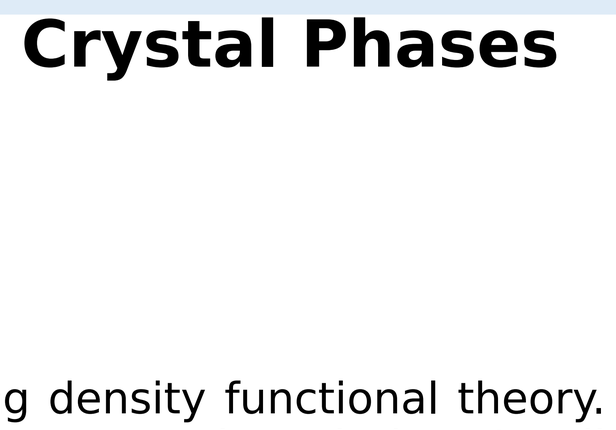
Bi Fe O

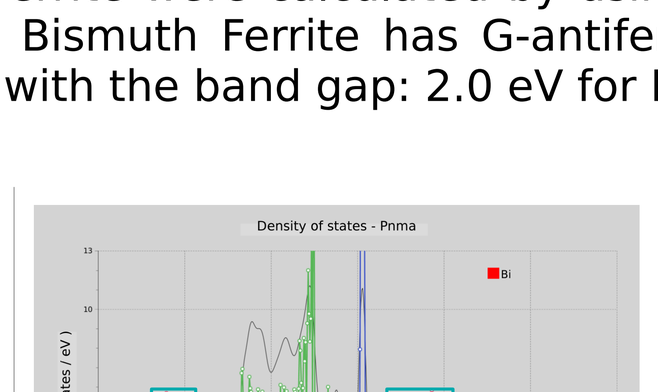
Results

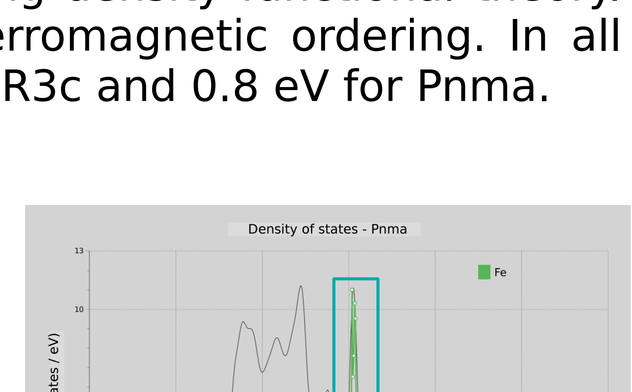












Conclusions

1) In the pnma phase it is observed that in the fermi level there is a high density of Fe states, so it can be said that it presents a metallic behavior

2) In the r3c phase, the states of the different elements are highly mixed in both the valence band and the conduction band.

References

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