First principle study on the effect of Mn substitution in NaFeAs

Mesfin Asfaw, Mark Pederson*
**Adama Science and Technology University, Adama, Ethiopia . mesfingn171@gmail.com*
The University of Texas at El Paso, Department of Physics

ABSTRACT

This work present the study on the effect of Mn substitution in NaFeAs applying density functional theory(DFT) as implemented in quantum ESPRESSO. In order to investigate this effect, 50% Mn-substitution on Fe site of NaFeAs were done. The band structure and the density of states(DOS) are calculated for non-magnetic (NM) and collinear-magnetic orderings. Comparison was done between (NaFeAs and $NaFe_{0.5}Mn_{0.5}$ As). The calculated band structures indicates that there is a significant change due to Mn in AFM ordering, where the two bands are completely different at the first Γ-point and in between the second Γ-point and the first Z-point. The DOS result shows that the Fe states dominated in the vicinity of the E_F , with only a small contribution from the As and Na. Using the DOS value and some approximation for BCS type, the Tc were calculated for NaFeAs and we obtained T c = 9.33k. The DOS in the presence of Mn decreases for AFM ordering and it seems that the effect of Mn on 1111-family is not similar with 111-family of IBSC. The calculated magnetic moment indicated that the material has a Ferii magnetic behavior.

Introduction

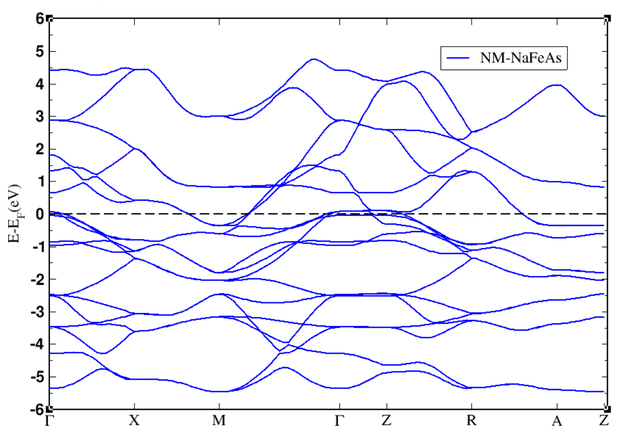
The study on iron based superconductors has been produced a large number of results since the report on $LaFeAsO_{0.89}F_{0.11}$[1,2]. NaFeAs is one of the 111-family superconductors that shows different properties up on substitution. NaFeAs is a superconductor without any impurity. It is also reported that substitutions of Fe by Co, Ni and Cu destroy the magnetic order and enhance Tc. But the positive effect of Mn is not yet reported. On the other hand Mn has a suppression effect on LaFeAsO [3,4]. In this work we tried to see the effect of Mn substitution on NaFeAs.

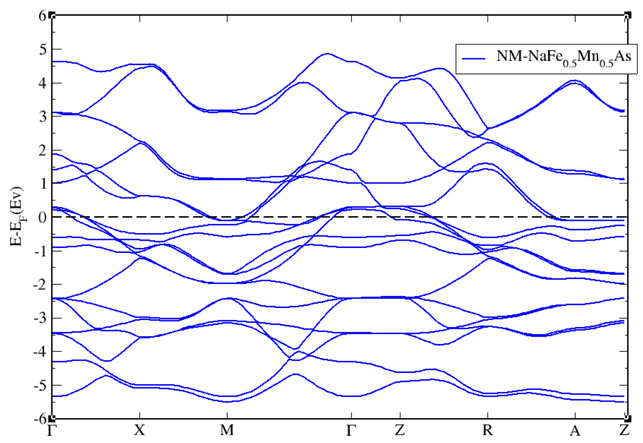
COMPUTATIONAL DETAILS

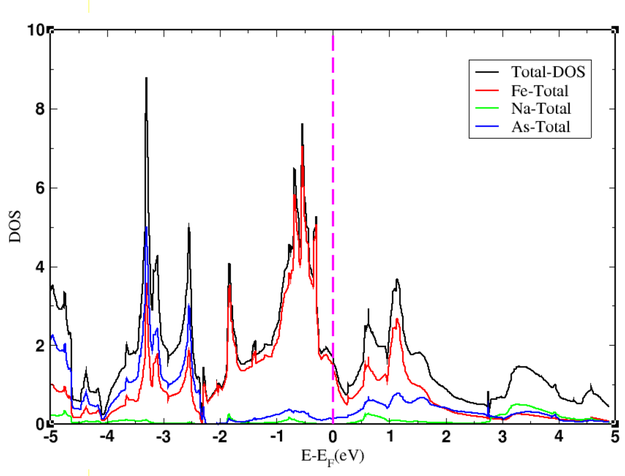
We apply first principle calculation (DFT) with Quantum ESPRESSO code[5]. We use the experimental value of the tetragonal lattice parameter, a and c. The bands are plotted along the high symmetry direction (Γ-X-M-Γ-Z-R-A-Z) in the Conventional Tetragonal-TET Brillouin zone[6]. we used k-mesh(8 8 5) and Ecut=60Ry. We did non magnetic and magnetic calculations.

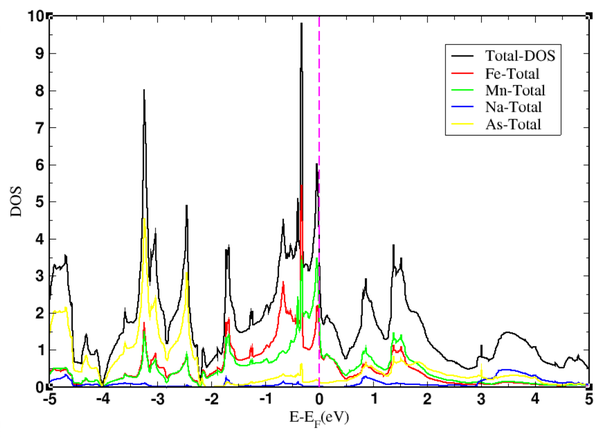
Results

a)Non magnetic calculation



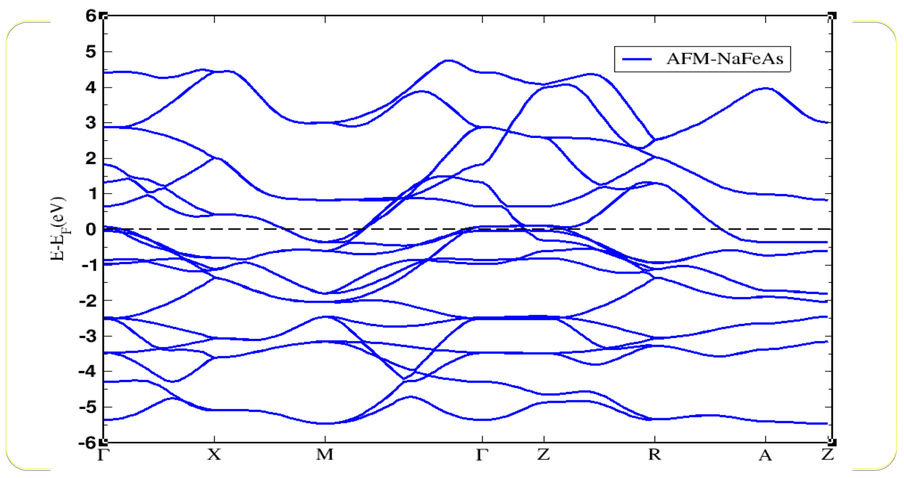


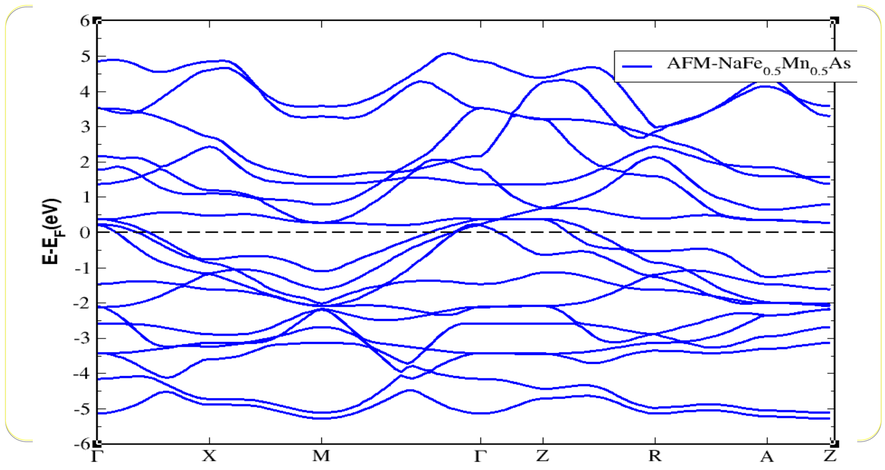


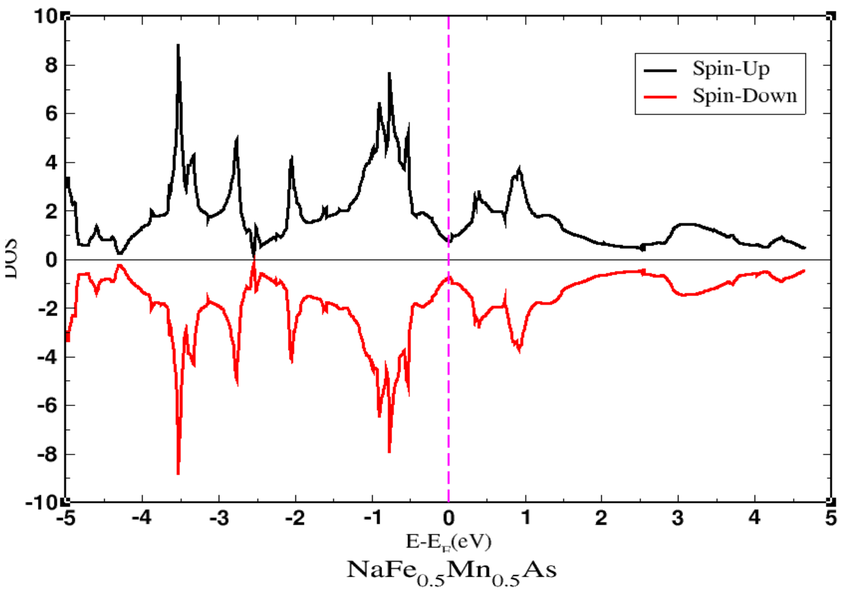


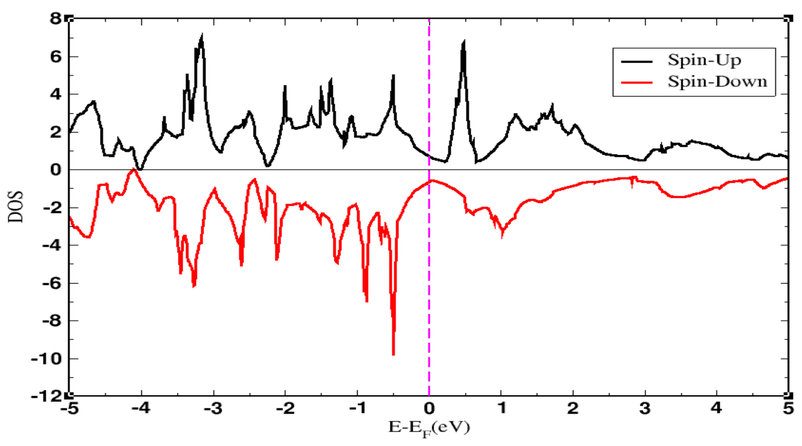
Critical temperature:
Tc = 9.33K (NaFeAs)
Tc = 8.4K ($NaFe_{0.5}Mn_{0.5}As$)
Magnetic moment:
In the presence of Mn(0.5) magnetic moment of Fe is increased
FM- 0.0017 to 2.0626
AFM- 0.0041 to 1.5634

b) Antiferomagnetic ordering









References

[1] Kamihara et al., J. Am. Chem. Soc. 130, 3296 (2008)
[2] G. R. Stewart, Rev. of Modern Phys. 83, 2011
[3] F. Hammerath et al., Phys. Rev. B 89, 134503 (2014)
[4] F. Hammerath, Phys. Rev B 97, 054522 (2018)
[5] P. Giannozzi et al., J.Phys.:Condens. Matter 21 395502 (2009)
[6] Wahyu et al Computational Materials Science 49 (2010) 299–312

The author wishes to acknowledge the organizations who supported participation in the 2022 Workshop on Recent Developments in Electronic Structure:

- the US-Africa Initiative in Electronic Structure (USAfrI)
- the Innovation Fund of the American Physical Society
- Columbia University
- and the East African Institute for Fundamental Research.