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Ab Initio Study of Magnetism in FeSe and FeTe

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Abstract. Magnetism in FeSe and FeTe systems is studied using density functional theory. Nonmagnetic (NM), ferromagnetic (FM) and three different antiferromagnetic (AFM) states are considered. We have investigated chalcogen height dependence of magnetism using LDA and GGA exchange correlations. For FeSe, LDA used for both structural optimization and magnetism, yields magnetic energies that seem close to experiments. For FeTe, LDA and GGA give different magnetic ground states for experimental z_{Te}. For FeTe, GGA gives magnetic ground state that is found in experiments, which is in contrast to FeSe and pnictides.

Keywords: DFT, magnetism, Fe based superconductors, exchange correlations
PACS: 74.70.Xa, 75.10.Lp, 72.20.Pq, 71.15.Mb

INTRODUCTION

The iron chalcogenides belong to interesting class of ferrous superconductors. These materials consist of stacking layers of Fe-X (X=Se and Te) along **c**-axis which plays key role in superconductivity [1]. In contrast to pnictides they do not have charge reservoir layers in addition to superconducting Fe-X layers and thus have advantage of structural simplicity. FeSe do not have any long range magnetic ordering and has superconducting transition temperature of around 8K [1]. FeTe is known to have double stripe [2, 3] type AFM ordering and do not exhibit any superconducting transition. Both magnetism and superconductivity in FeSe is very sensitive to stoichiometry. Perfectly stoichiometric FeSe being nonmagnetic and superconducting [4], any deficiency or excess of Fe results in ferri/ferromagnetism [5, 6]. Density functional calculations based upon pseudopotential based method by Chang et. al. [7] shows that it is height of chalcogen atoms above Fe-Fe planes that drives magnetism in these systems. However, from DFT point of view these systems are quite sensitive to approximations used and tiny details of structure due to itinerant nature of magnetism in these materials [8]. We have here carried out Full Potential Linear Augmented Plane Wave (FPLAPW) [9] method based DFT calculations for FeSe and FeTe and found that not only chalcogen height but nature of chalcogen have crucial role in the magnetism of these systems. Also exchange correlation is quite important. Whereas LDA seems to be suitable for FeSe, it fails for FeTe to produce experimentally observed double stripes type magnetic ground state and one has to use GGA for this system. This type of situation is not encountered in pnictides.

COMPUTATIONAL DETAILS

All the calculations are performed using full potential linear augmented plane wave (FPLAPW) method as implemented in WIEN2k code [9]. The muffin tin radii of $2.00a_0$ for Fe, Se and $2.10a_0$ for Te are used. The calculations of total energies in different magnetic states are done for more than 100 k-points in IBZ. We have ensured convergence of total energy with different parameters such as number of plane waves, maximum value of angular momentum etc.

STRUCTURAL DETAILS

Both FeSe and FeTe crystallize in tetragonal structure with spacegroup *P4/nmm*. Fe is located at 2a site (0.75, 0.25, 0.00) and Se/Te at 2c site (0.25, 0.25, z). The experimental values of lattice parameters for FeSe [1] and FeTe [10] are taken. The height of chalcogen above Fe-Fe planes is used in accordance with Chang et. al. [7] and defined as $h=z\times\mathbf{c}$, where **c** is length of **c** axis. Different magnetic states considered are nonmagnetic (NM), ferromagnetic (FM) and three different AFM states known as single stripes (SS), double stripes (DS) and checkerboard (CH). These states are illustrated in reference [7] by Chang et. al.

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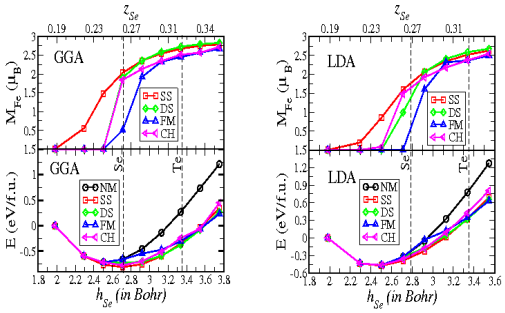

Figure 1 Total energy of FeSe vs. h_{Se} above Fe planes

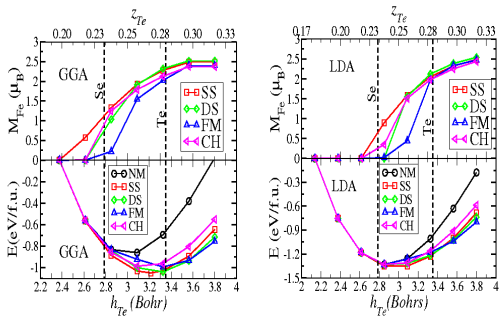

Figure 2 Total energy of FeTe vs. h_{Te} above Fe planes

RESULTS AND DISCUSSIONS

Total energy and magnetic moment on Fe as a function of height (h) of chalcogen above Fe planes for FeSe and FeTe is given in Figures 1 and 2 respectively. The dashed lines correspond to experimental values of Se and Te in FeSe and FeTe respectively. For comparison, we have used LDA and GGA. The minima of total energy curves correspond to minimum force positions and are consistent with force minimization results. It is interesting to notice that for SS state Fe retains its magnetic moment up to much lower heights than other magnetic states.

TABLE 1. Results of force minimization using GGA, experimental values are in brackets

	h (a.u.)
FeSe (in NM state)	2.5159 (2.7861)
FeTe (in DS state)	3.2960 (3.3515)

For FeSe, at experimental and optimized value of h_{Se}, SS is the ground state. Though, for experimental value energetic stability of SS is around 200meV/Fe which is quite large. For optimized value the energetic stability of SS state is 47meV/Fe in GGA and 10meV/Fe for LDA. The dynamical effects like spin fluctuations can suppress the magnetic ordering of the states which have 10-15meV/Fe energy stability [8]. Thus GGA overestimates magnetic energies in FeSe and one must use LDA to explain no long range magnetic ordering in FeSe. Experimental value of h_{Te} comes in region where double stripes (DS) state is ground state for FeSe in both LDA and GGA.

For FeTe, at experimental h_{Te} using LDA we got that SS is the ground state whereas using GGA we obtained DS as the ground state. Experimentally, it is found that FeTe has DS as the ground [2, 3]. Thus one must use GGA for FeTe in order to explain the experimental results. At optimized value of h_{Te}, we found that there is a crossover from DS to SS, below which SS is the ground state.

Thus despite of having same structure and Se and Te being isoelectronic, FeSe can only be described by LDA and FeTe can only be described by GGA. These findings are interesting and seek attention from theoretical point of view.

CONCLUSION

In conclusion we have investigated magnetism in FeSe and FeTe as function of height of chalcogen atoms above Fe planes. We found that for FeSe to justify experimental observations, one should use NM relaxed structure using LDA/GGA and then should use LDA to calculate magnetic energies. This is in contrast to FeTe where one has to use experimental atomic positions and GGA for magnetism to produce experimentally observed magnetic ground state.

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REFERENCES

1. F.C. Hsu et. al. Proc. Natl. Acad. Sci. USA (2008) Sep 23;105(38):14262-4
2. F. Ma et. al. Phys. Rev. Lett. 102, 177003, (2009)
3. W. Bao et. al. Phys. Rev. Lett. 102, 247001 (2009)
4. T.M. McQueen et. al. Phys. Rev. B 79, 014522 (2009)
5. X. J. Wu et. al. J. Appl. Phys. 103, 113501 (2008)
6. K.-W. Lee et. al. Phys. Rev. B 78, 174502 , (2008)
7. Chang Y. et. al. Phys. Rev Lett. 104, 057003 (2010)
8. I. I. Mazin et. al. Phys. Rev. B 78, 085104 (2008)
9. P. Blaha et. al. WIEN2k, An Augmented Plane Wave+Local Orbitals Program for Calculating Crystal Properties (Technical University of Vienna, Vienna, 2001)
10. VPS Awana et. al. Physica C 471, 77 82 (2011)