Density Functional Study of Perovskite Superconductor MgCNi3

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Density Functional Study of Perovskite Superconductor $MgCNi_3$

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Abstract. We here report the first principle density functional study of $MgCNi_3$ which crystallize in cubic perovskite structure having critical transition temperature of 8K. The interesting aspect of this compound is that in normal state it is non magnetic in nature despite conduction electrons in it are derived from partially filled Ni d states, which typically lead to ferromagnetism in metallic Ni and many Ni-based binary alloys. To investigate the detailed microscopic origin of the non magnetic nature we have done density functional based calculations on this compound. The lattice constant is calculated using minimum energy criteria from total energy versus lattice constant plot. By taking the calculated values of lattice constant we have done the precise calculations on the compound using Full Potential Linear Augmented Plane Wave (FP-LAPW) method implemented in ELK code. The electronic density of states is found spin degenerate that corresponds to a non-magnetic ground state. The density of states (DOS) at Fermi level, $N(E_F)$ is dominated by Ni-d states. The sharp peak observed just below Fermi level corresponds to van Hove singularity (vHs). The projected density of states (PDOS) suggests a strong hybridization of Ni-3d and C-2p states which is responsible for the observed non magnetic nature of $MgCNi_3$.

Keywords: DFT, GGA, DOS, ELK, vHs
PACS: 71.15.Mb, 74.25.Jb, 74.70.Ad

INTRODUCTION

The discovery of superconductivity in perovskite structure $MgCNi_3$ is of special interest as it has provided a link between two major families of superconducting materials namely inter-metallic compound, MgB_2 and perovskite based non-cuperate materials, $Ba_{1-x}K_xBiO_3$ [1]. The surprising aspect is the presence of large amount of Ni in the unit cell, the element that is mostly associated with magnetism. The observance of superconductivity in Ni based compounds is however not unprecedented as the quaternary borocarbides ($RENi_2B_2C$) [2], binary alloy of Bi and Ni (Bi_3Ni) [4], etc. are some of the known nickel based superconductors. The interesting part in $MgCNi_3$ is that in normal state it is non magnetic in nature despite conduction electrons in it are derived from partially filled Ni-d states [5], which typically lead to ferromagnetism in metallic Ni and many Ni-based binary alloys. To investigate the detailed microscopic origin of non-magnetism we have performed density functional based calculations on this material. As a precursor to understand the magnetic nature we have done the calculations for $MgCNi_3$ and carbon removed hypothetical compound $MgNi_3$ to show that C-p orbitals has strong hybridization with Ni-d orbitals that leads to spin degenerate electronic density of states in $MgCNi_3$.

COMPUTATIONAL DETAILS

The calculations were performed using density functional based approach employing Full Potential Linear Augmented Plane Wave (FP-LAPW) basis as implemented in ELK code [6]. The Brillouin zone integrations were performed using 15x15x15 mesh containing 120 k-points. The values of Muffin tin radii for Mg, C and Ni were 2.00, 1.45 and 2.00 a.u. respectively. We used generalized gradient approximation [7] for solids (GGA PBEsol) to describe the exchange and correlation for the system. The lattice constant for $MgCNi_3$ was determined by plotting total energy versus lattice constant and was found to be 7.12 a.u. which is within 1.1% of experimental value 7.20 a.u. The compound $MgCNi_3$

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was found to converge to a non-magnetic ground state. However, calculations on hypothetical $MgNi_3$ lead to a magnetic state with its equilibrium lattice constant of 6.72 a.u. The comparison of $MgNi_3$ and $MgCNi_3$ suggests that C in octahedral site not only expands the lattice but also arrests the formation of Ni-local moments due to strong hybridization effects.

RESULTS AND DISCUSSION

Fig.1 shows the total and site resolved electronic density of states (DOS) for experimental lattice constant of $MgCNi_3$. The DOS for both spins is found exactly overlapped that shows non-magnetic nature of the compound. The value of DOS at Fermi-level is found to be 102.5 states/Hartree-Cell (3.79 states/eV-Cell) which is in good agreement with calculations reported in literature [8]. The atom resolved DOS shows that most of the states near Fermi level arise from Ni-d states and Mg and C states are relatively small at Fermi-level. The bonding Mg-s states (not shown here) are distributed from 0.1 to 0.26 Hartree below Fermi-level that shows covalent bonding with Ni-d orbital whereas, corresponding anti-bonding orbitals are found from 0.04 to 0.4 Hartree above Fermi level.

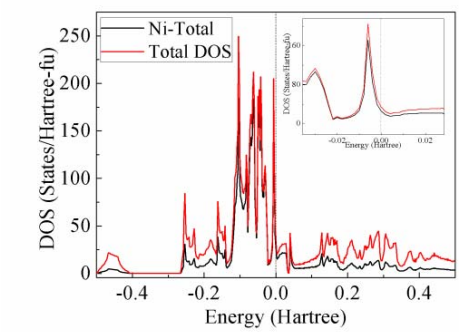

Figure 1 Electronic Density of States of $MgCNi_3$ and contribution of total Ni states

Fig. 2 depicts the *l* and *m* resolved DOS for Ni and C atoms. It is observed that C-s states lie approximately 0.4 Hartree below Fermi-level, whereas C-p states are found from 0.3 to 0.1 Hartree below Fermi-level. C-p states can also be found around Fermi-level that shows the hybridization of these states with Ni-d states which are dominating at Fermi-level. The Ni states were observed mainly from Ni-d orbitals as was seen from *l* and *m* resolved DOS. The characteristic feature of the DOS is sharp peak just below Fermi-level mainly containing Ni-d states. This peak represents a van Hove singularity (vHs) like feature which is also seen in certain high temperature superconductors HTSCs. Mazin and Singh [5] have emphasized that this vHs leads to Stoner enhancement that can lead to spin fluctuations in $MgCNi_3$.

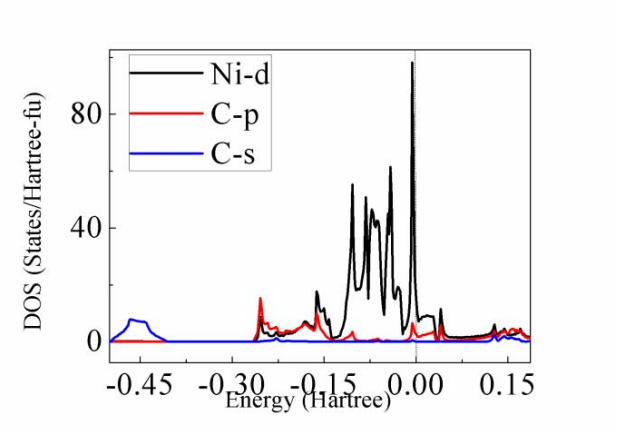

Figure 2 *l* and *m* resolved DOS for Carbon and Nickel in $MgCNi_3$

The calculations done on hypothetical compound $MgNi_3$ for experimental lattice constant of $MgCNi_3$ resulted in the magnetic ground state with magnetic moment of $1.12\mu_B$ that corresponds to 0.37 μ_B per Ni atom that is slightly less that the value for bulk Ni (0.61 μ_B per Ni atom).

CONCLUSION

In conclusion we have studied perovskite superconductor $MgCNi_3$ using density functional theory. We have found that C-p orbitals undergo strong hybridization with Ni-d orbitals leading to non magnetic nature.

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