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First-Principle Study of Electronic Structure and Magnetic Properties of Tb_2FeCrO_6

Sarita Lawaju[1,2], Shalika Ram Bhandari[1,2], Santosh K. C.[3], and Madhav Prasad Ghimire[1,2*]

[1]Central Department of Physics, Tribhuvan University, Kirtipur, 44613, Kathmandu, Nepal
[2]Condensed Matter Physics Research Center, Butwal-11, Rupandehi, Nepal
[3]San José State University, San Jose, California, United States

* madhav.ghimire@cdp.tu.edu.np

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Abstract

Electronic and magnetic properties of Tb_2FeCrO_6 (TFCO) is investigated using density functional theory (DFT). TFCO shows the insulating property with the band gap of 0.048 eV and 2.372 eV with generalized gradient approximation (GGA) and GGA + U respectively. The antiferromagnetic configuration, AFM1 [$Fe_1Fe_2Cr_1Cr_2$-↑↓↑↓] is found to be the ground state. Further, exchange coupling constants $J_{Cr\text{-}Cr}$(-0.99 meV), $J_{Fe\text{-}Fe}$ (-5.68 meV), and $J_{Cr\text{-}Fe}$ (-1.36 meV) are calculated to get depth knowledge on magnetic realm of TFCO.

Keywords: Density functional theory; generalized gradient approximation; antiferromagnetic; magnetic exchange interaction

Introduction and Motivation

- Double perovskite (DP) is the compound having general formula $A_2BB'O_6$, where A – rare earth element; B,B' - transition elements.
- DPs containing Fe and Cr shows interesting properties like multiferroicity and can have varieties of applications.[1]
- Experimentally, TFCO showed re-entrant spin reorientation and griffith's phase transition.[2]
- TFCO-Pbnm structure has G-type antiferromagnetic ground state and shows insulating property.[2]
- Spin-Heisenberg Hamiltonian: $\hat{\mathbf{H}}_{\mathbf{spin}} = -\sum_{\mathbf{i<j}} \mathbf{J_{ij}} \hat{\mathbf{S}}_{\mathbf{i}} \hat{\mathbf{S}}_{\mathbf{j}}$

[1]P. Baettig, and N. A. Spaldin, Appl. Phys. Lett., **86**, 012505, (2015)

[2]B. Mali, H. S. Nair, *et. al.,* Phys. Rev. B, **102**, 014418, (2020)

Crystal Structure

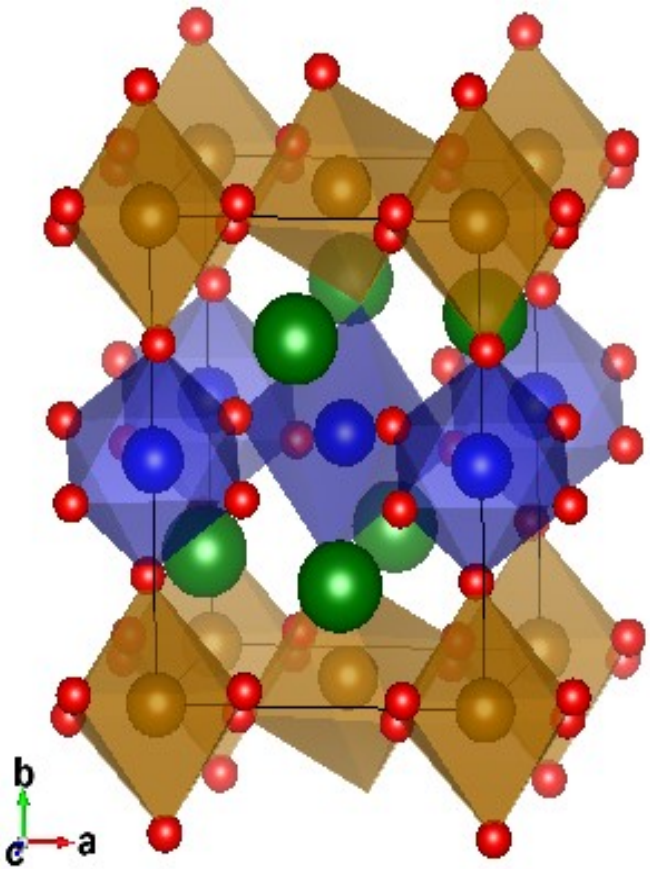


Figure: Crystal structure of Tb_2FeCrO_6 (Pnma)

- Tb_2FeCrO_6 - space group (62 - Pnma), orthorhombic
- Lattice parameters:
  a = 5.53913 Å, b = 7.59173 Å,
  c = 5.31242 Å and
  α = β = γ = 90°
- Charge state: Tb ($4f^8$) ⟶ +3,
  Fe ($3d^5$) ⟶ +3,
  Cr ($3d^3$) ⟶ +3
- Neel's temperature (experimental):
  - T_N = 257 K
- $S_{Fe} = \frac{5}{2}$, $S_{Cr} = \frac{3}{2}$

Computational Details

- Used density functional theory (DFT) using FP-LAPW + lo method implemented in WIEN2k code.[3]
- R_{MT} values for Tb, Fe, Cr and O are 2.35, 2.0, 1.96 and 1.72 Bohr respectively.
- Implemented generalized gradient approximation (GGA) and hubbard potential (+U).
- On-site potential values used are: U_{Tb} = 6 eV, U_{Fe} = 5 eV, and U_{Cr} = 3 eV.
- Self-convergence criteria: energy convergence – 10^{-5} Ry, charge convergence – 10^{-4} e.
- 6 X 6 X 6 k – mesh over irreducible Brillouin Zone (BZ).

[3]P. Blaha *et. a*l., WIEN2k, 2001.

Results and Discussions

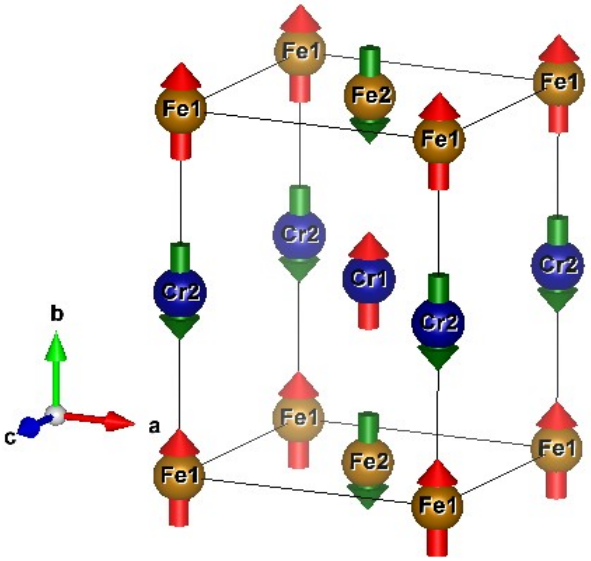


Figure: Ground state spin configuration of TFCO-Pnma

- Optimized position of 3d-transition elements is in order $Fe_1Fe_2Cr_1Cr_2$.
- Up/down spins of magnetic ions Fe_1, Fe_2, Cr_1, Cr_2 ordering are:
  FM-↑↑↑↑ , AFM1-↑↓↑↓ , AFM2-↑↓↓↑ ,
  FIM1-↑↑↓↓ , FIM2-↑↓↓↓
- **Spin ground state configuration** - AFM1- ↑↓↑↓ (G-Type AFM).

- Magnetic moments: Fe(GGA) = ± 3.67 μ_B, Cr(GGA) = ± 2.36 μ_B
  Fe(GGA+U) = ± 4.12 μ_B, Cr(GGA+U) = ± 2.57 μ_B
- Present of band gap of 0.048 (2.372) eV within GGA (GGA + U).

Results and Discussions

Density of States (DOS)

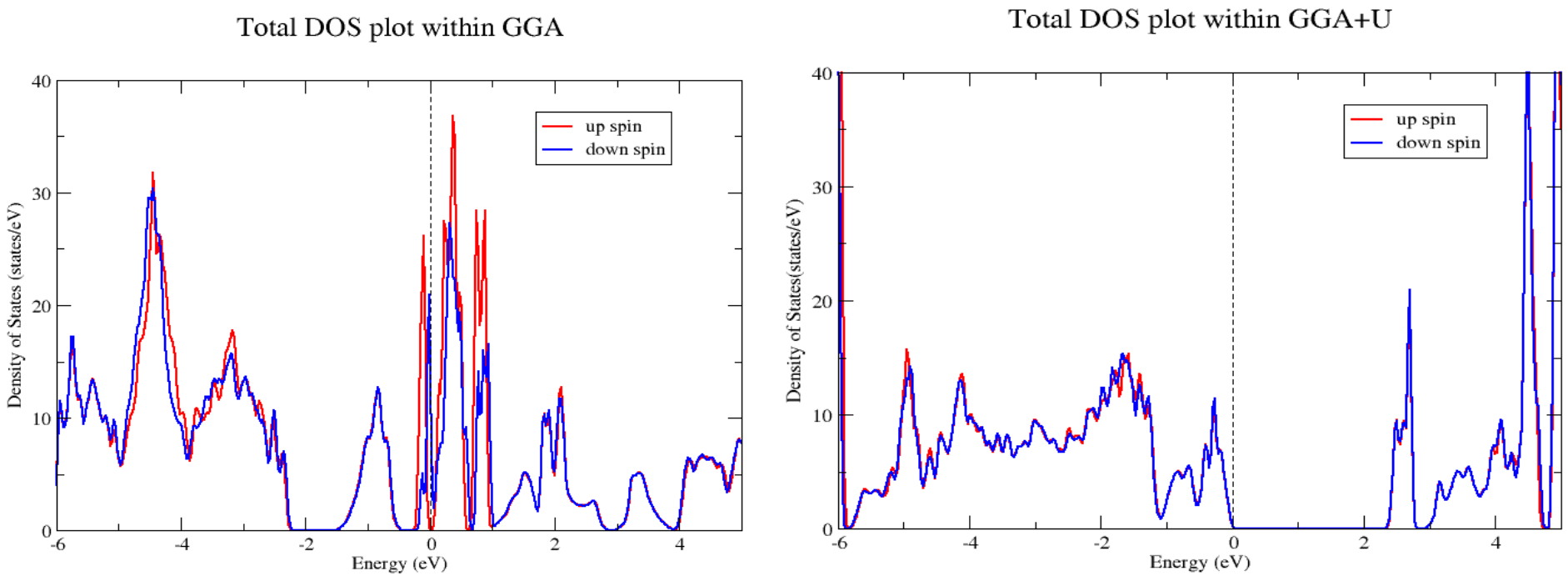


Figure: Total DOS plots of Tb_2FeCrO_6 within GGA (left) and GGA + U (right)

- Gap has increased after applying on-site potential (U), pushing away localized orbitals.
- Compound shows perfect anti-ferromagnetism after applying +U

Results and Discussions

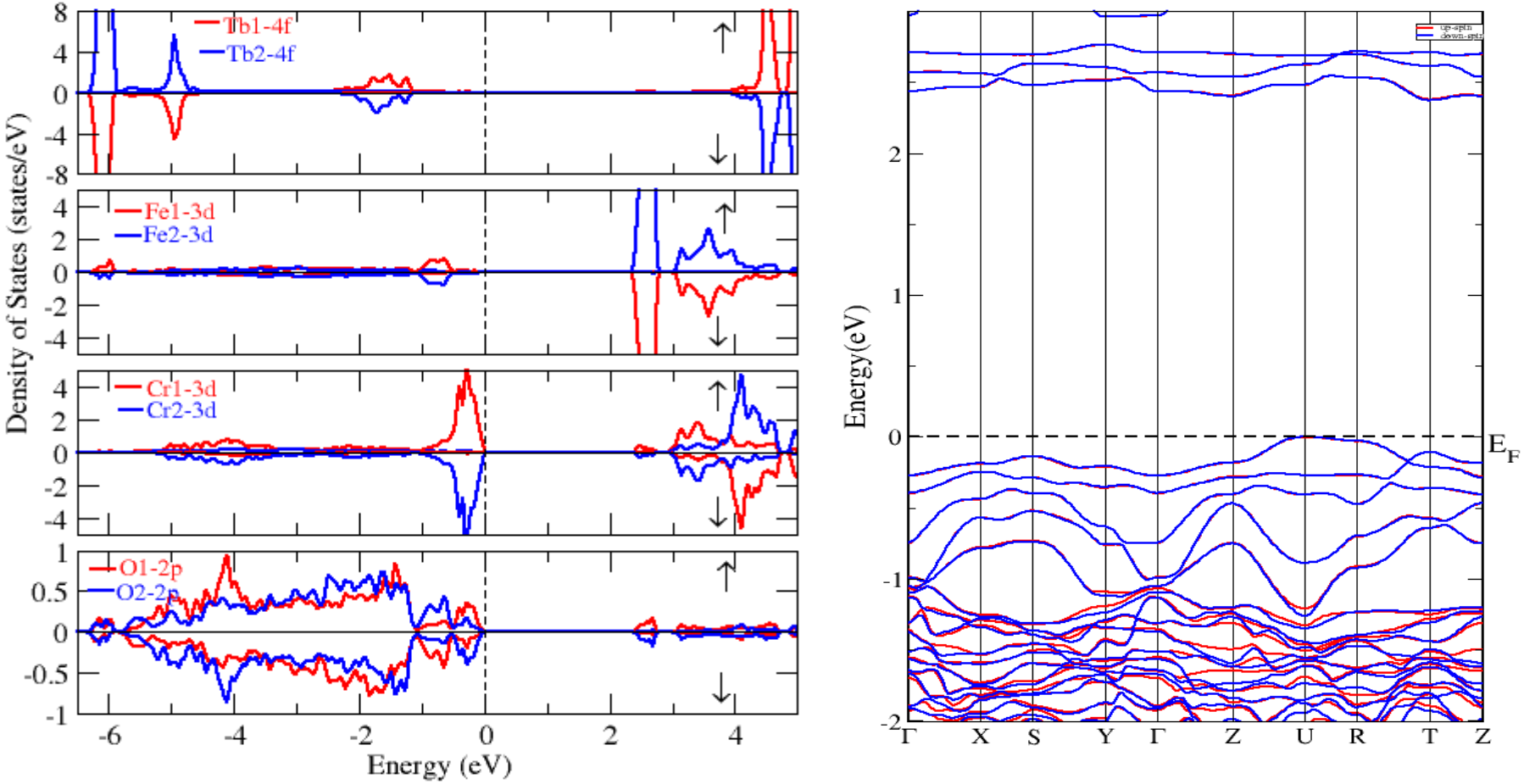


Figure: Partial DOS (left) and band structure (right) within GGA + U

- Band gap is increased from 0.048 eV (GGA) to 2.372 eV (GGA+U).
- Gap is contributed by Cr-3d (valence region) and Fe-3d (conduction region).

Results and Discussions

Exchange coupling constants

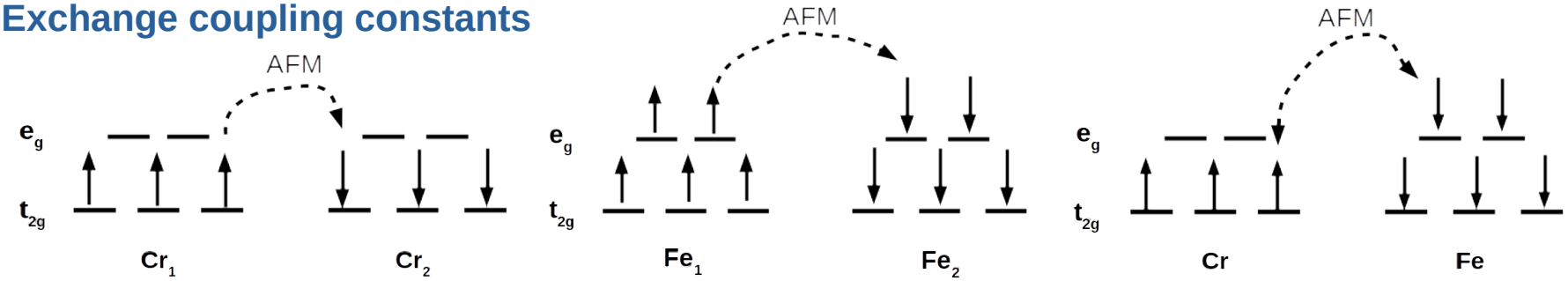


Figure: Super-exchange interactions between Cr atoms (left), Fe atoms (middle) and Cr-Fe atoms (right)

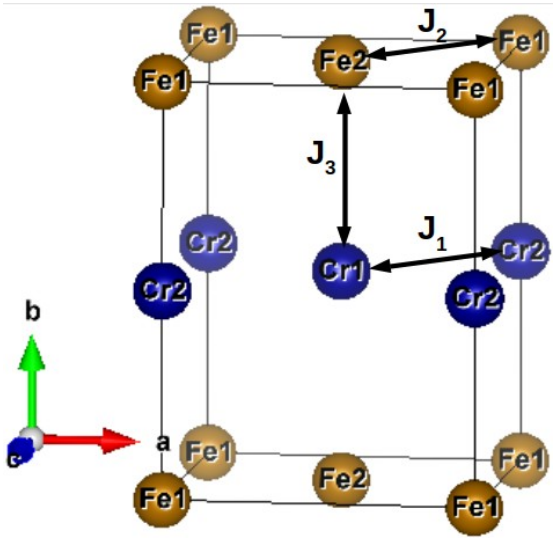


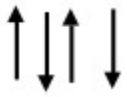
Figure: J – path chosen for TBCO

- $J_{Cr\text{-}Cr}$ = -0.99 meV: Anti-ferromagnetic order.
- $J_{Fe\text{-}Fe}$ = -5.68 meV: Anti-ferromagnetic order.
- $J_{Cr\text{-}Fe}$ = -1.36 meV: Anti-ferromagnetic order.
- The interaction between Fe atoms is stronger of all.
- Neel's temperature was theoretically calculated using formula:

$$T_N = \frac{2S_{Fe}S_{Cr}}{3K_B}(4J_1 + 4J_2 + 2J_3)$$

- T_N(calculated) = 853.69 K

Conclusions

- G – Type AFM1-  [$Fe_1Fe_2Cr_1Cr_2$] is the spin ground state.
- Compound is an insulator with a band gap of 0.048 (2.372) eV within GGA (GGA+U).
- Gap is contributed by Cr-3d and Fe-3d states
- The exchange interactions between all transition elements are in antiferromagnetic order.
- Insulating behavior of compound shows possibilities of Multiferroicity in it and hence potential uses in spintronic devices, photo-voltaic devices, memory states, etc.

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