Electronic and Magnetic Properties of Co-doped $Rb_2Ni_3S_4$

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Outline

- Introduction/Background
- Methodology and Computational tools
- Electronic and magnetic properties of $Rb_2Ni_3S_4$
- Half metallicity in Co-doped $Rb_2Ni_3S_4$
- Discussion and Conclusions

Introduction/Background

Kagome Metals

- Kagome: Traditional Japanese woven bamboo pattern.
- Japanese Word : Kago - Basket, Me - Eyes.
- Atoms of a conducting substances arranged in Kagome pattern - shows exotic electronic properties.
- Kagome lattice: Vertices and edges of tri-hexagonal tiling, each hexagon is surrounded by triangles.
- Importance : conduct electricity without losing energy at room temperature.

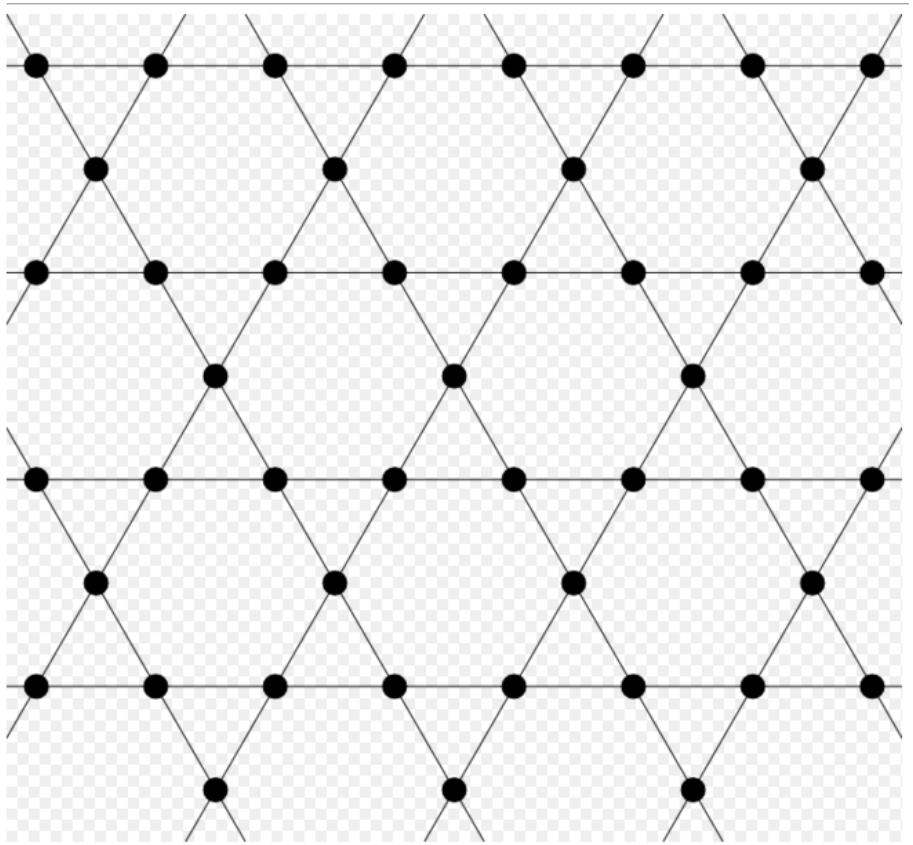

Figure: structure of kagome lattice. [a]

[a] http://www.hfmphysics.com/2006/motif.

Introduction/Background

Half Metals

- One spin channel metallic.
- Opposite spin channel insulating.
- Zero energy band gap superior electronic properties than non zero energy gap material.
- Importance: Practical applications in spintronics, electronics and sensors.

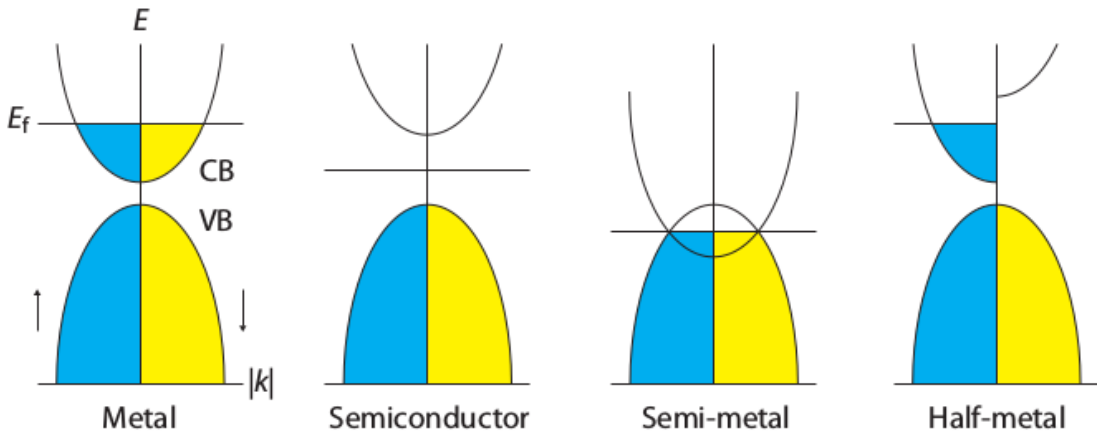

Figure: The electronic band structures of various classes of materials. [1]

[1] (Wang *et al., NPG Asia Mater.* ***2****, 31, (2010)*

Crystal structure $Rb_2Ni_3S_4$

- Face centered-orthorhombic structure with the space group *Fmmm* (69)
- Symmorphic space group
- lattice parameters: a = 5.90615070 Å, b = 10.06449278 Å, c = 13.43457036 Å
- Angles : $\alpha = \beta = \gamma$ = 90°

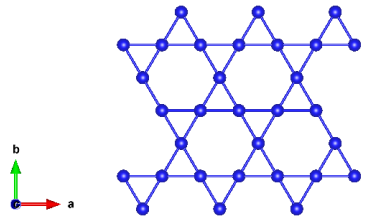

Figure: Ni ions constitute a Kagome lattice

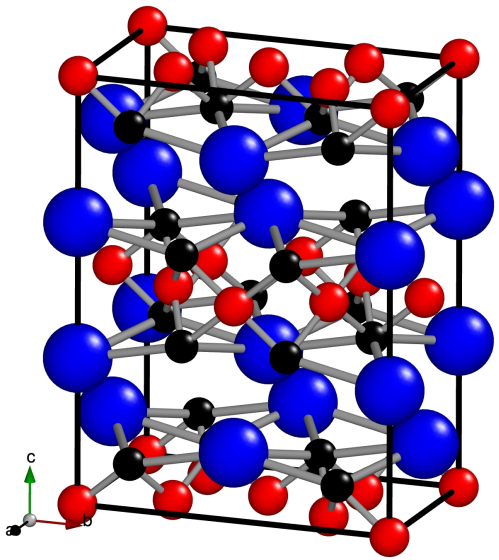

Figure: Crystal structure of $Rb_2Ni_3S_4$. (blue balls are Rb atoms, red balls are Ni atoms and black balls are S atoms)

Methodology and Computational tools

- Study electronic and magnetic properties of $Rb_2Ni_3S_4$ and Co-doped $Rb_2Ni_3S_4$ Density functional theory (DFT)calculation.
- Generalized gradient approximation (GGA) used for exchange correlation interaction.
- Full Potential Local Orbital (FPLO)code used for calculations.

Results and Discussion

Electronic and Magnetic Properties of $Rb_2Ni_3S_4$

- Nonmagnetic, ferromagnetic and antiferromagnetic configuration.
- Ground state is to be weak ferromagnetic.

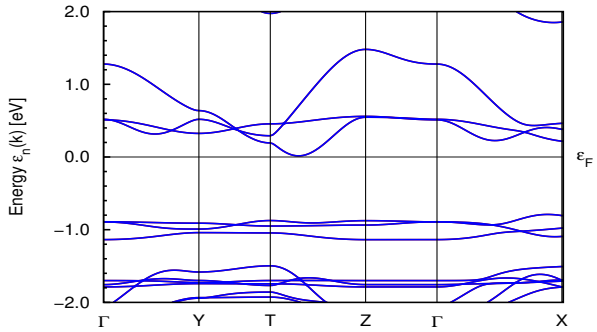

Figure: Band structure of $Rb_2Ni_3S_4$ in scalar relativistic.

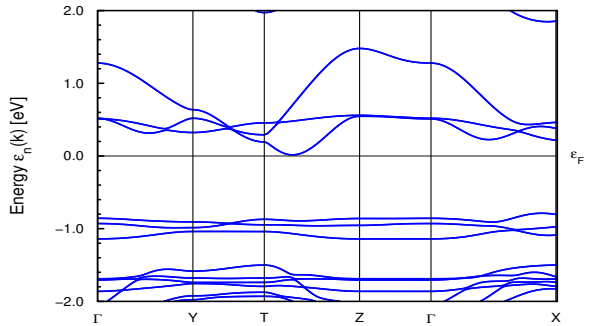

Figure: Band structure of $Rb_2Ni_3S_4$ in full relativistic.

Results and Discussion

Electronic and Magnetic Properties of Co-doped $Rb_2Ni_3S_4$

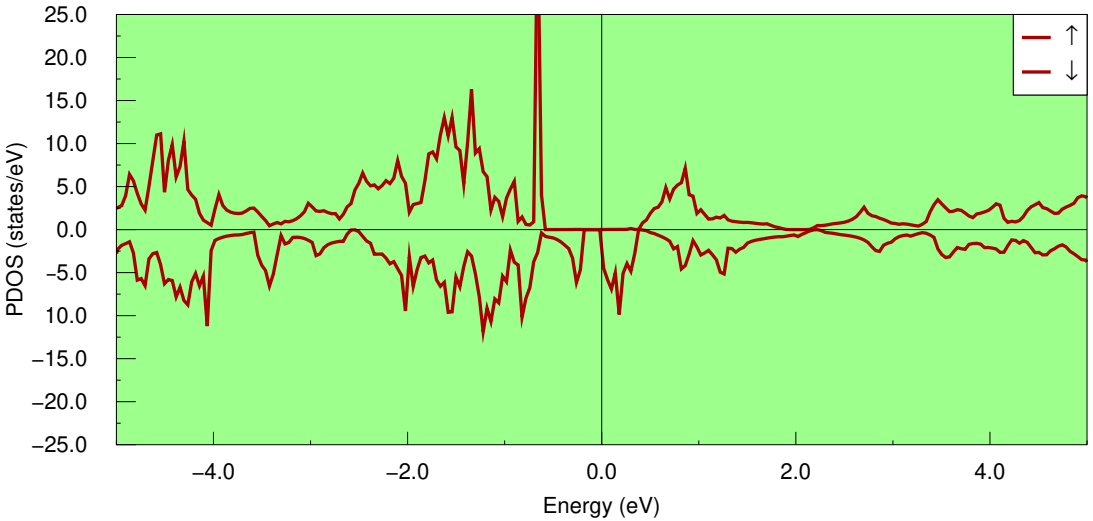

Figure: Density of states of Co-doped $Rb_2Ni_3S_4$ in scalar relativistic

- Co-doped in the place of first Ni.
- Ground state is ferromagnetic.

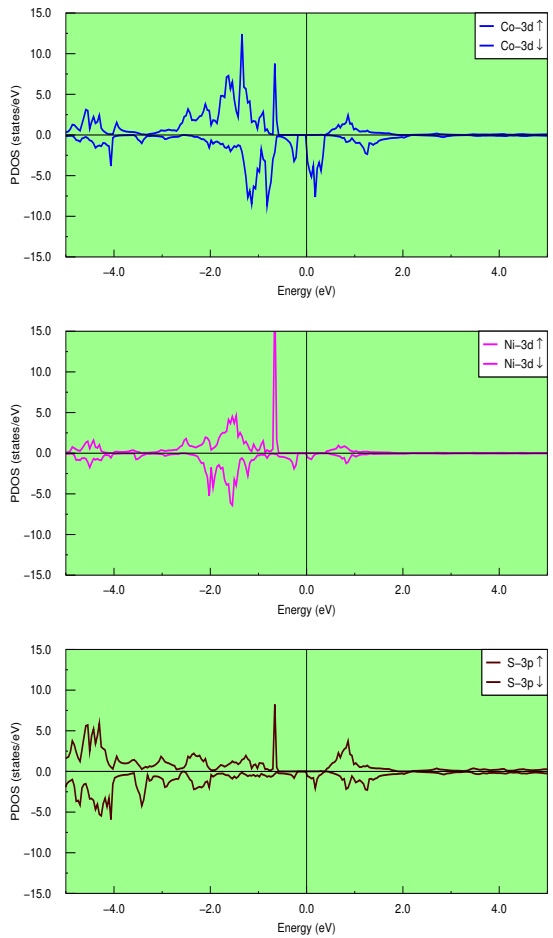

Figure: Partial Density of states of Co-doped $Rb_2Ni_3S_4$ in scalar relativistic.

Results and Discussion

Electronic and Magnetic Properties of Co-doped $Rb_2Ni_3S_4$

- Half metallic ferromagnetism.
- magnetic moment 2.0μ_B /unit cell.
- Ferromagnetism mainly derived from Co-3d spins.
- Strong hybridization between Ni-3d and Co-3d orbitals.

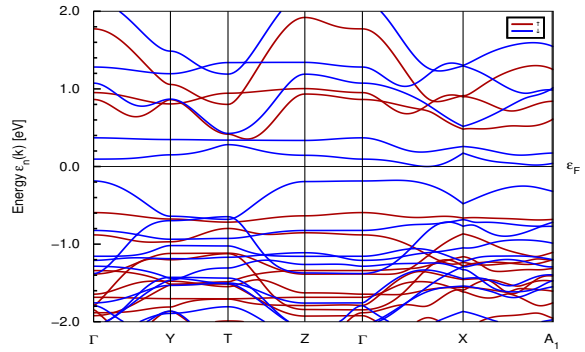

Figure: Band structure of Co-doped $Rb_2Ni_3S_4$ in scalar relativistic

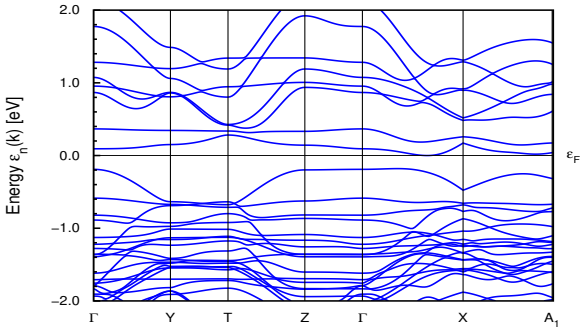

Figure: Band structure of Co-doped $Rb_2Ni_3S_4$ in full relativistic

Electronic and Magnetic Properties of Co-doped $Rb_2Ni_3S_4$

- Kagome lattice materials can host flat band.
- With energy 0.36eV above the Fermi level.
- Electronic flat bands in momentum space arising from strong localization of electrons.

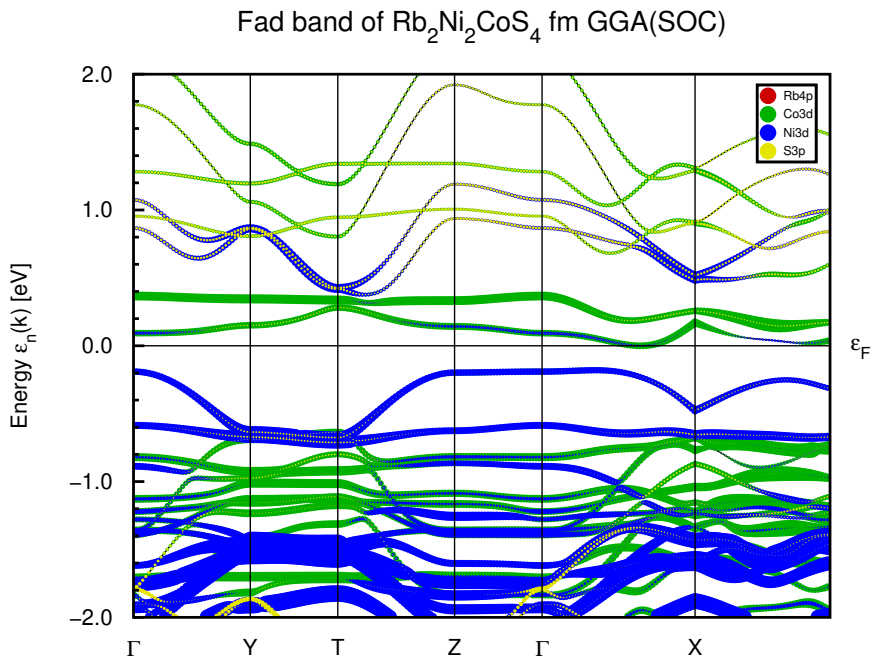

Figure: Fad band structure of Co-doped $Rb_2Ni_3CoS_4$ in full relativistic

Conclusions

- Parent materials $Rb_2Ni_3S_4$ is weak ferromagnetic in nature.
- Upon full replacement of Ni(1) by Co atom ferromagnetic half metallic state achieved.
- Strong hybridization between Ni 3d and Co 3d orbitals.

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Thank
You!