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Effect of Hole Doping in Kagome System YCo_5

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Abstract

With the presence of robust flat band in YCo_5, which has high Magnetocrystalline Anisotropy Energy (MAE) among itinerant magnets, doping of hole with smaller ionic radii to the Y-site has shown significant change in the MAE. This system is found to be pseudo two dimensional ferromagnetic in nature under density functional calculations employing GGA+U exchange potential in WIEN2k. With hole doping the original flat band is extended to whole Brillouin zone. In addition to it the Fermi level is shifted because of it. This enables to control the filling of flat bands upon doping, resulting in novel feature of band engineering.

Keywords: Kagome magnet; Magnetocrystalline Anisotropy Energy; Density Functional Theory; Exchange interaction; Flat band

Introduction

- Magnets
  - Energy generation, storage
  - **Green Energy** unprecedented growth in demand
  - Ever increasing demand and constrained cost

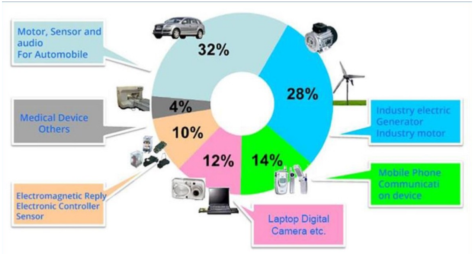

Fig: Uses of Permanent magnets (*www.tcd.ie/Physics/research/groups/magnetism*)

- The choice of materials is limited to include magnetic elements only
- Rare-earth based magnets including $Nd_2Fe_{14}B$ and intermetallic magnet $SmCo_5$ $\rightarrow$ champion hard magnets.
- YCo_5 **mishmetal** highest anisotripy energy and Curie temperature required for the permanent magnets among itinerant magnets [1].

[1] K. Ohashi, *Nippon Kinzoku Gakkai-Shi* **76** (2012)

- Rare-earth free magnets
  - Low cost and more cost efficient than rare-earth magnets
  - Tunable magnetization direction in absence of rare-earth [2]
  - High magnetization and Curie temperature becaue of transition metals
- Ytterium based magnets
  - High anisotropy and susceptibility is less effected by temperature [3]
  - Anti-parallel coupling of Y-*d* electrons with *d* electrons of transition metals [4]
  - Doping on Y-site to enhance the MAE without changing the contribution from *Co* atoms
  - Tunable magnetization direction

[2] M. Matsumoto, R. Banerjee, and J. B. Staunton *Phys. Rev. B* **90** (2014)

[3] B. Szpunar, *Physica B+ C* **130** (1985)

[4] K. Strnat, G. Hoffer, J. Olson, W. Ostertag, and J. J. Becker, *Journal of Applied Physics* **38** (1967)

Methodology

- Electronic and magnetic structure calculations are done by employing Density Functional Theory (DFT).
- WIEN2k based on Full Potential Linearized Augmented Plane Wave (FP-LAPW) is used as the tool for DFT [5]
- Standard Generalized Gradient Approximation (GGA) was employed as exchange functional
- Supercell approach was used for the fractional doping on Y-site

[5] P. Blaha, K. Schwarz, G. K. H. Madsen, D. Kvasnicka, and J. Luitz, Technische Universität Wien, Vienna, Austria, (2001)

Structure of YCo_5

- The kagome system YCo_5 belongs to hexagonal $CaCu_5$ structure, with three inequivalent sites for Y(1a), Co(2c) and Co(3g).

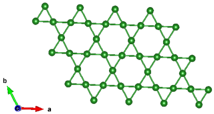

Fig: Kagome arrangement Co(3g)

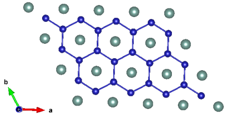

Fig: Hexagonal arrangement Co(2c)

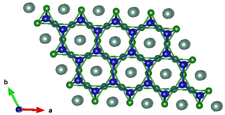

Fig: Planer structure YCo_5

- In ground state Y aligns itself in opposite direction (with low induced moment) with ferromagnetic arrangement of *Co* atoms

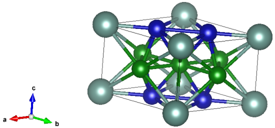

Fig: Crystal structure YCo_5 (where gray balls are Y, green balls are Co(3g) and blue balls are Co(2c))

Density of States plots

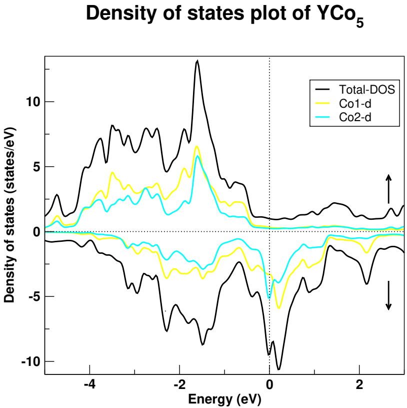

Fig : Density of states of parent compound YCo_5

- Spin down → Co(2c) (**major**) with Co(3g)
- Spin up → Co (3g) and a little from Co(2c)
- The magnetic moments obtained

	GGA	GGA+U
Y (1a)	-0.20 μB	-0.25μB
Co (2c)	1.57 μB	1.85 μB
Co(3g)	1.60 μB	1.91 μB
Total	7.20 μB	8.10 μB

- Since *Co* on YCo_5 is in intermediate spin state we have taken the value of on-site potential $U = 3\ eV$ throughout this work

DOS and band plots

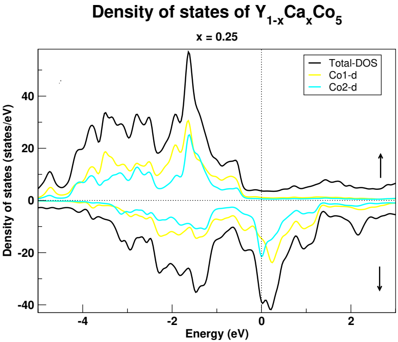

Fig: Density of states of $Y_{0.75}Ca_{0.25}Co_5$

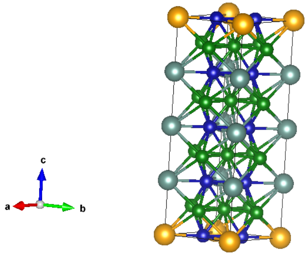

Fig: $Y_{0.75}Ca_{0.25}Co_5$ crystal

- **Observed magnetic moment in μB of $Y_{0.75}Ca_{0.25}Co_5$**

	Y	Ca	Co(3g)	Co(2c)	Total
GGA	-0.20	-0.10	1.71	1.58	31.08
$+U = 3\ eV$	-0.22	-0.11	1.97	1.91	34.32

DOS and band plots

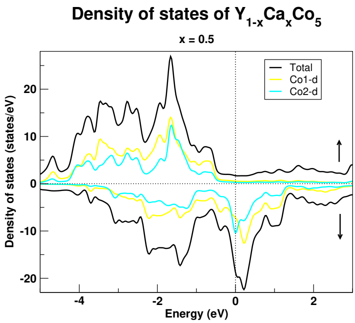

Fig : Density of states of $Y_{0.5}Ca_{0.5}Co_5$

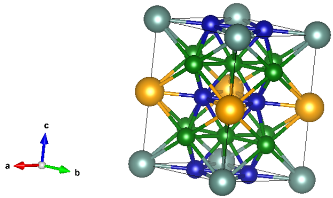

Fig : $Y_{0.5}Ca_{0.5}Co_5$ crystal

- **Observed magnetic moment in μB of $Y_{0.50}Ca_{0.50}Co_5$**

	Y	Ca	Co(3g)	Co(2c)	Total
GGA	-0.17	-0.07	1.74	1.65	15.22
$+U = 3\ eV$	-0.13	-0.06	1.96	1.91	17.22

DOS and band plots

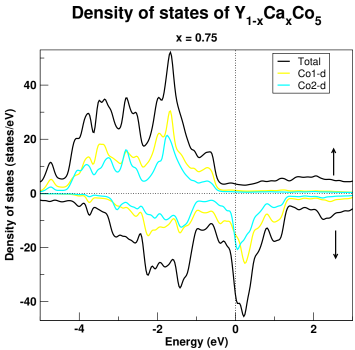

Fig : Density of states of $Y_{0.25}Ca_{0.75}Co_5$

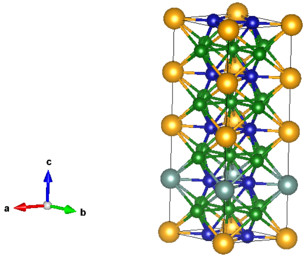

Fig : $Y_{0.25}Ca_{0.75}Co_5$ crystal

- **Observed magnetic moment in μB of $Y_{0.25}Ca_{0.75}Co_5$**

	Y	Ca	Co(3g)	Co(2c)	Total
GGA	-0.20	-0.10	1.72	1.64	29.52
$+U = 3\ eV$	-0.17	-0.07	1.98	1.93	35.71

Band plots

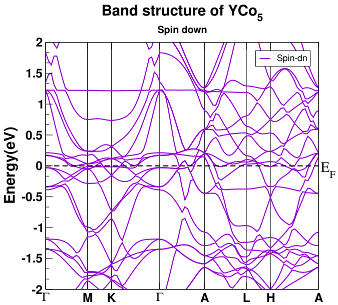

Fig : Spin down of YCo_5

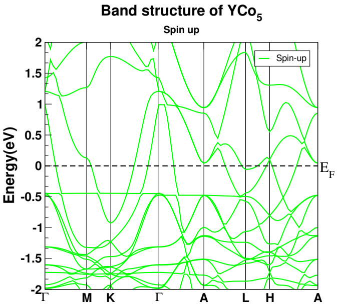

Fig : Spin up of YCo_5

- Flat band is present in path $\Gamma - M - K - \Gamma - A$ in both spin-channels
- $E_F = 0.6095\ eV$

Band plots

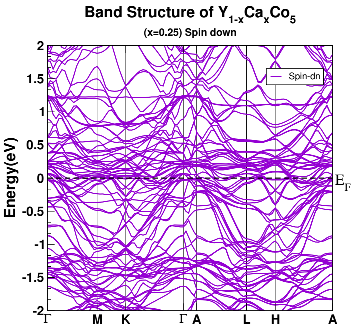

Fig : Spin down of $Y_{0.75}Ca_{0.25}Co_5$

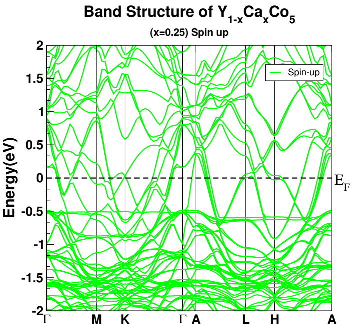

Fig : Spin up of $Y_{0.75}Ca_{0.25}Co_5$

- Flat band is present in path $\Gamma - M - K - \Gamma - A$ in both spin-channels
- Another flat band is also seen in $A/L - L - H - H/A$
- $E_F = 0.5464\ eV$

Band plots

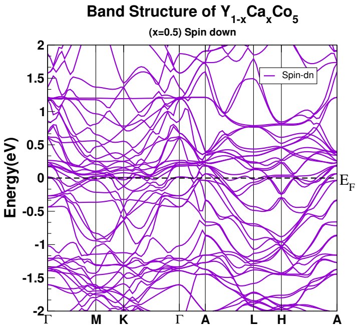

Fig : Spin down of $Y_{0.5}Ca_{0.5}Co_5$

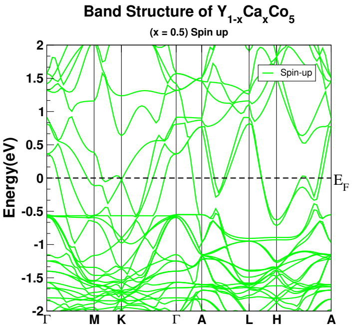

Fig : Spin up of $Y_{0.5}Ca_{0.5}Co_5$

- Flat band is present in path $\Gamma - M - K - \Gamma - A$ in both spin-channels
- $E_F = 0.5476\ eV$

Band plots

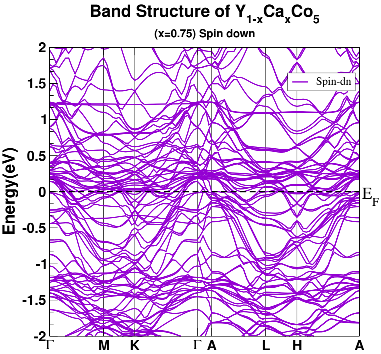

Fig : Spin down of $Y_{0.25}Ca_{0.75}Co_5$

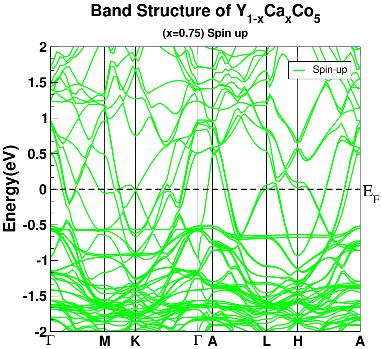

Fig : Spin up of $Y_{0.25}Ca_{0.75}Co_5$

- Flat band is present in path $\Gamma - M - K - \Gamma - A$ in both spin-channels
- Another flat band is also seen in $A/L - L - H - H/A$
- $E_F = 0.6095\ eV$

Conclusions

- We investigated $Y_{1-x}Ca_xCo_5$ with (x =0,0.25,0.50 and 0.75) using DFT
- $Y_{1-x}Ca_xCo_5$ for all values of x are ferromagnets
- Magnetocrystalline Anisotropy Energy is found to decrease with increase in the concentration of dopant *i.e Ca*
- The Fermi level shifted downwards with increase in the concentration of *Ca*
- Flat band shifted away from Fermi level with increased doping for spin up and in case of spin down channel it shifted towards fermi level

Acknowledgments

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- Ministry of Social Development, Gandaki Province, Nepal