Electronic and Magnetic Properties of Kagome Metal $MgFe_6Ge_4$

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Abstract

Wide range of investigation is going on to study kagome lattice to create device with perfect conductivity. Here, we perform density functional calculation using FPLO code to study electronic and magnetic properties of $MgFe_6Ge_4$, a kagome system, where we noticed the material to be ferromagnetic with a total magnetic moment of 11.38 μ_B/unit cell. We found the metallic nature where Fe-3d shows the highest contribution at Fermi level in total DOS. Hybridization between Fe-3d and Ge-4p is observed around Fermi level. The Wannier fitting with the DFT calculations was performed to obtain wannier Hamiltonian to explore the Weyl points in $MgFe_6Ge_4$.

Keywords: Kagome lattice; Density functional theory

Crystals
2020

Introduction

Kagome Metal

➔ **Word kagome derived from japanese kagome basket**

➔ **Two dimensional network of corner-sharing triangle**

➔ **Exhibit novel properties like anamolous hall effect, quantum anamolous hall effect**

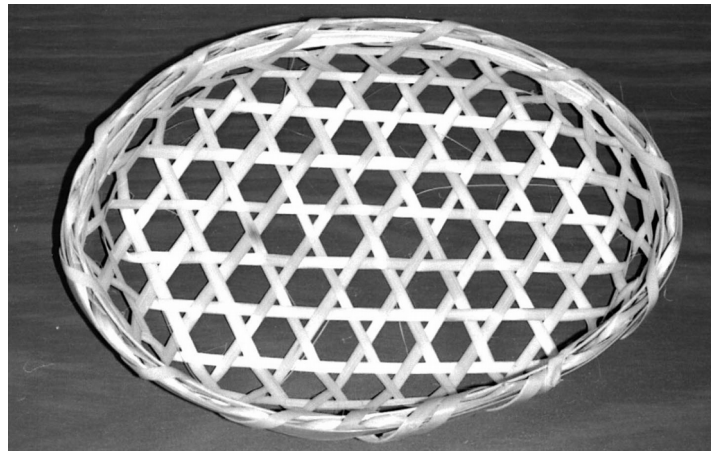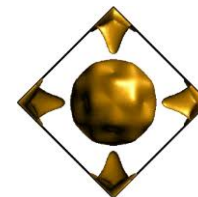➔ **Possibility of metals with kagome lattice in quantum computing**

Fig 1: Bamboo basket woven in kagome pattern
Physics today (2003)

Computational Methods

- **Density Functional theory calculation is performed in the full-potential local orbital code (FPLO).**

  K. Koepernik and H. Eschrig , Phy. Rev. B 59, 1743 (1999)

- **Scalar-relativistic and Full relativistic calculation was performed for 6 * 6 * 6 k-mesh.**

- **Standard generalized gradient approximation (GGA) is considered.**

- **Tight binding Hamiltonian is obtained by considering Wannier band mapping with FPLO.**

Results and Discussion
Crystal Information

- **Hexagonal Crystal**

- **Experimental lattice parameter**

- **$a=b=$ 5.09 Å, $c=$ 20.10Å**

  Matar *et al*., Solid State Sciences, (2015)

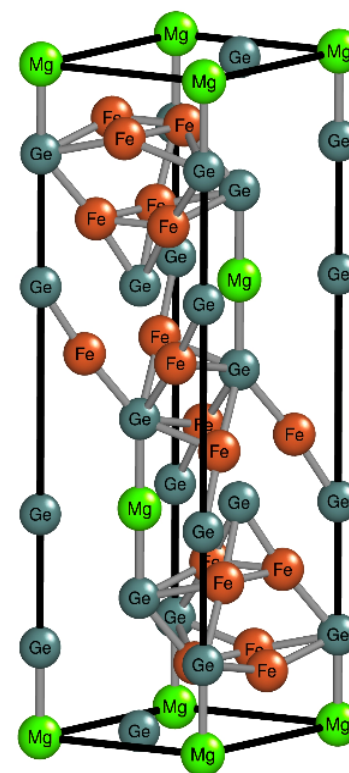- **α = β =90°, γ = 120°**

- **Space group: R$\overline{3}$m (166)**
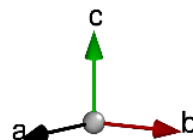
Fig 3: Crystal Structure of MgFe$_6$Ge$_4$
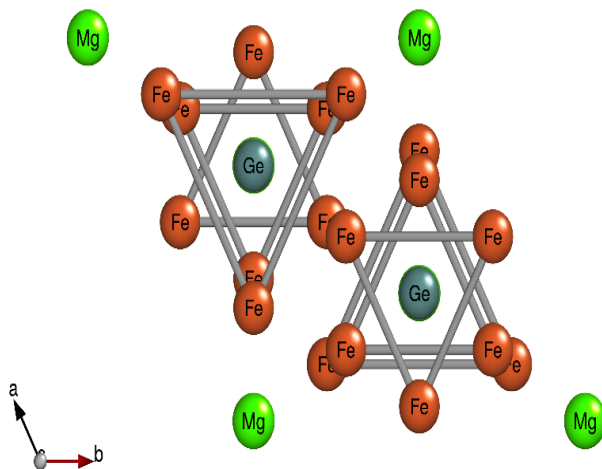
Fig 4: Kagome structure formed by Network of Fe atoms in MgFe$_6$Ge$_4$
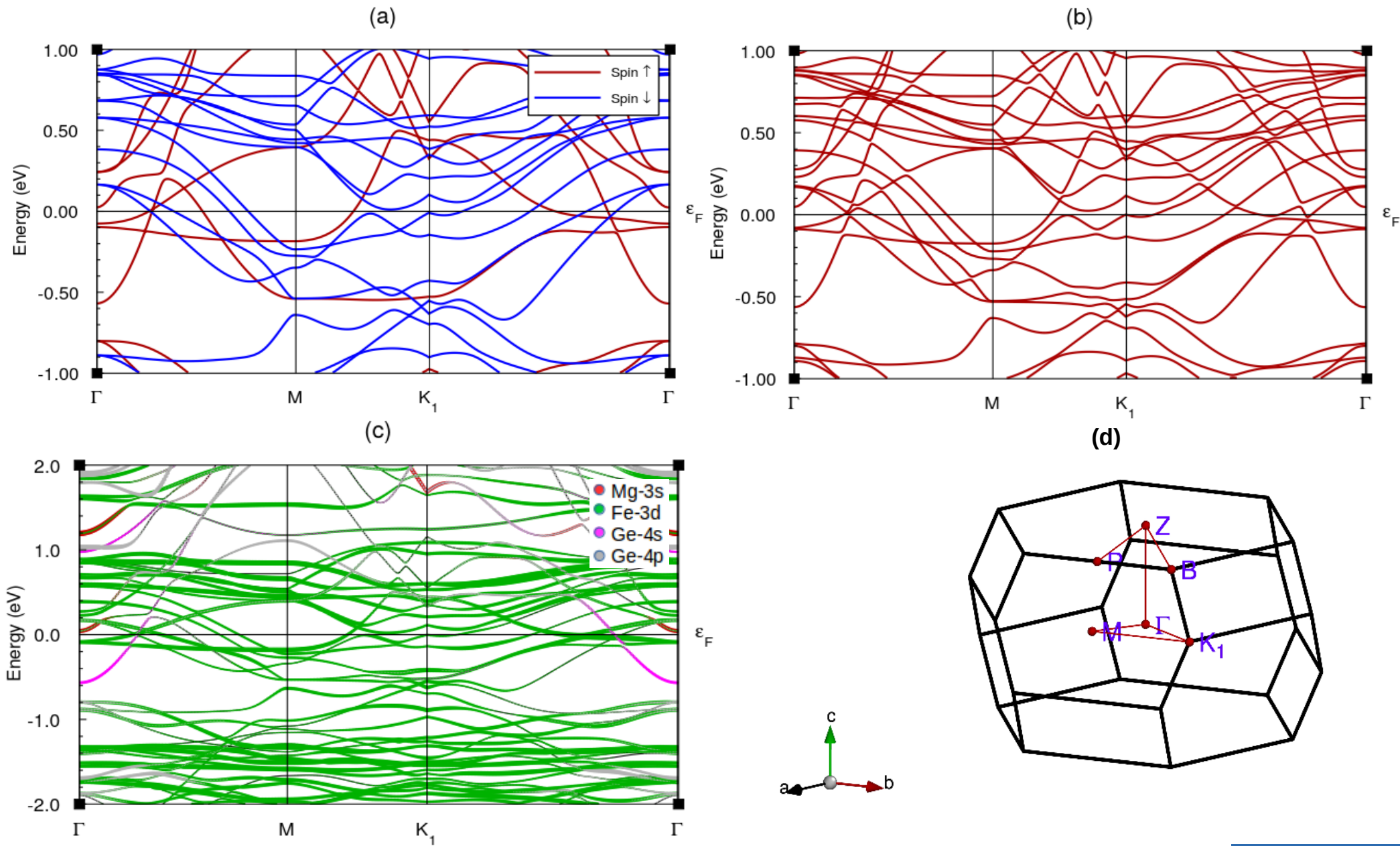
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Band Structure

Fig 7: Band Structure (a) Scalar relativistics, (b) Full relativistics (c) Contribution of Mg-3s, Fe-3d, Ge-4p, Ge-4s (d) Brillouin zone
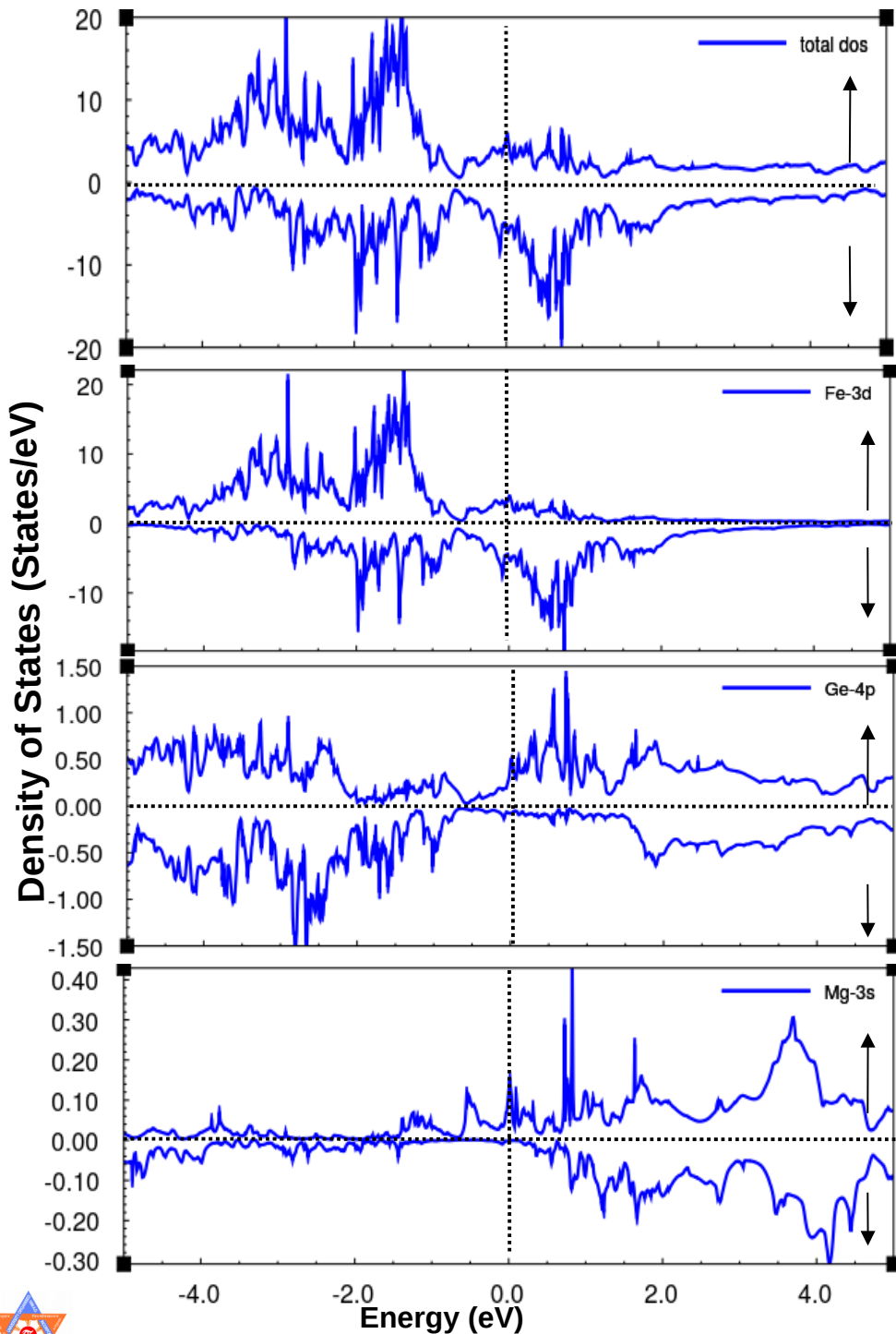
Electronic and Magnetic Properties

Fig 7: Density of States

☐ **Remarks**

→ **Fe-3d bands contribute mostly in the Fermi level.**

→ **Hybridization between Fe-3d and Ge-4p is observed at and around Fermi level.**

→ **$MgFe_6Ge_4$ is ferromagnetic material.**

☐ **From DFT calculations magnetic moment per unit cell**

$Fe(\mu_B)$	$Mg(\mu_B)$	$Ge_{average}(\mu_B)$	$\mu_{tot}(\mu_B)$
2.0680	-0.0230	-0.2512	11.3804

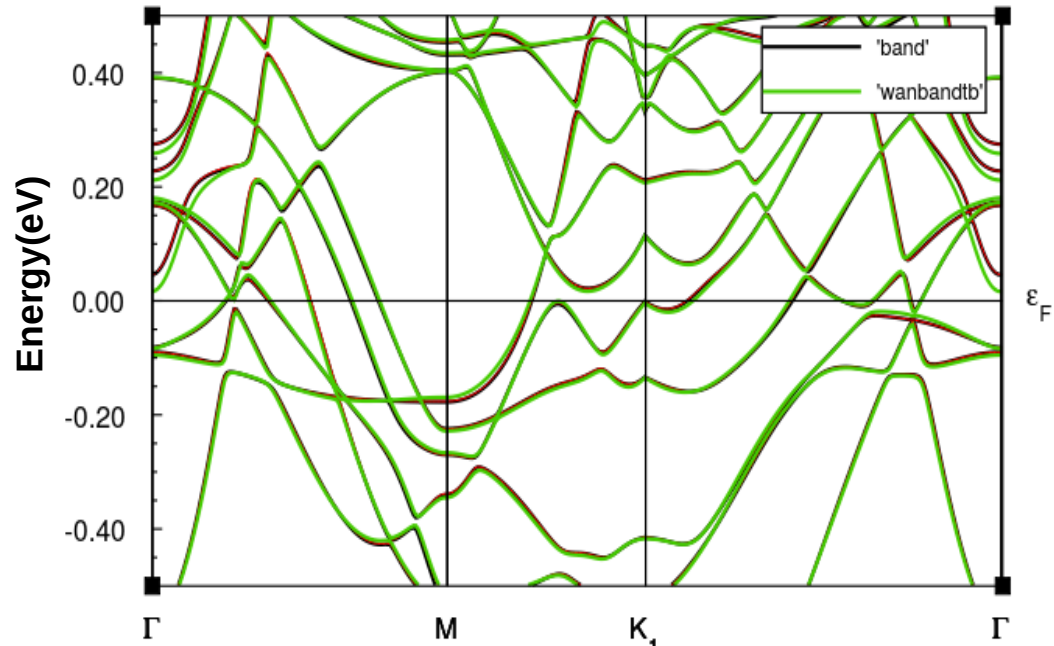Crystals 2020

Wannier Fitting

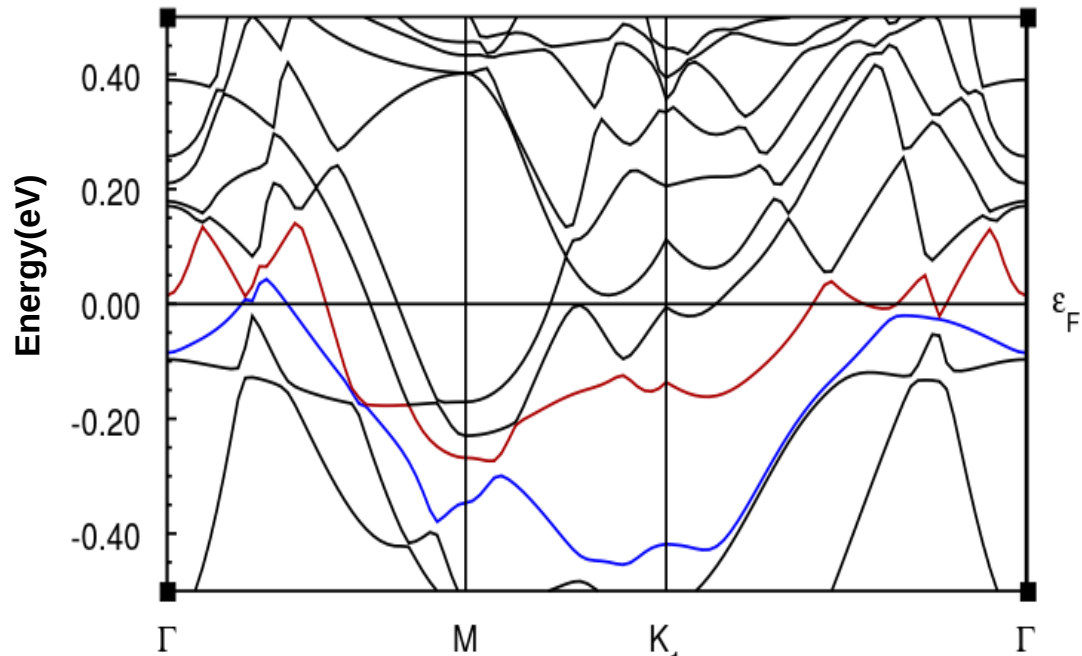Fig 9: Wannier band mapping

Fig 10: red band – CBM, blue band - VBM

Conclusions

- **MgFe$_6$Ge$_4$ is a ferromagnetic material found to be consistent with experiment.**

  Matar *et al*., Solid State Sciences, (2015)

- **Study of DOS and band structure shows MgFe$_6$Ge$_4$ is metallic compound.**

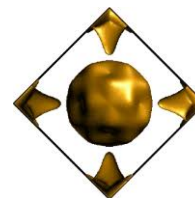- **Weyl crossing at Γ and M indicates Weyl semimettalic feature**

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→ **Kagome, Physics today, (2003)**

→ **K. Koepernik and H. Eschrig, Phy. Rev. B 59, 1743, (1999)**

→ **S. F. Matar *et al.*, Solid State Sciences, 39, 82, (2015)**

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