Electronic, Magnetic, and Optical Properties of Double Perovskites Pb_2XOsO_6 (X=Co, Ni)

Bishnu P. Belbase[1,2], Shalika R. Bhandari[1,2,3], Madhav P. Ghimire[1,2,3]

[1] *Central Department of Physics, Tribhuvan University, Kirtipur 44613, Kathmandu, Nepal*
[2] *Condensed Matter Physics Research Center, Butwal, Rupandehi, Nepal*
[3] *Leibniz Institute for Solid State and Materials Research Dresden, Helmholtz str. 20, 01069 Dresden, Germany*

Outline

- Introduction
- Methods and Computational Details
- Crystal Structure
- Results and Discussion
- Conclusions

Introduction

Materials Type

- Metals
- Half-metals
- Semiconductors
- Insulators

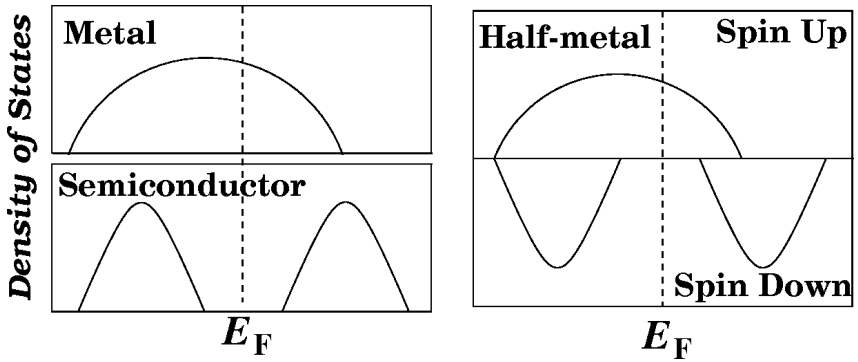

Fig: Classification of materials according to their energy gap [I. Galanakis *et al., arXiv preprint cond-mat/0510276 (2005)*]

Double Perovskites (DPs)

- Most common DPs are $A_2BB'X_6$
- DPs covers all types of materials
- Shows remarkable properties like structural stability, superconductivity, half-metallicity etc

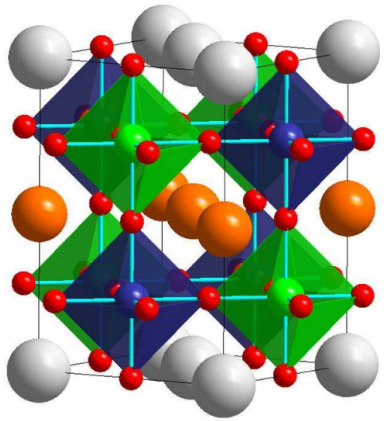

Fig: Ideal DPs structure [K. Momma *et al., J. Appl. Crystallogr.* ***44****, 1272 (2011)*]

Introduction

Applications

- Spintronics devices
- Photovoltaic application
- Laser light and light-emitting diode
- Microelectronics and telecommunication

Osmium based DPs

- $Sr_2CrOsO_6 \rightarrow$ Half metallic antiferromagnet [1]
- $Ba_2NiOsO_6 \rightarrow$ Dirac-Mott insulating ferromagnet [2]
- $Ca_2CrOsO_6 \rightarrow$ Ferrimagnetic insulator [3]
- $SrLaFeOsO_6 \rightarrow$ Metallic antiferromagnet [4]

---

[1] K. W. Lee *et al., Phys. Rev. B* ***77****, 115101 (2008)*
[2] H. L. Feng *et al., Phys. Rev. B* ***94****, 235158 (2016)*
[3] S. R. Bhandari *et al., RSC Adv.* ***10****, 16179 (2020)*
[4] D. K. Yadav *et al., Comput. Mater. Sci.* ***170****, 109168 (2019)*

Methods and Computational Details

Theoretical approach

- Performed density functional calculation to explore electronic and magnetic properties
- Used GGA functional
- GGA+U functional considered to account strong correlation effect of Co-3d, Ni-3d and Os-5d
- U-value for $Pb_2CoOsO_6 \rightarrow$ Co=4 eV and Os=2 eV
- U-value for $Pb_2NiOsO_6 \rightarrow$ Ni=5 eV and Os=2 eV

Computational details

- Full potential local orbital (FPLO) code is used for calculation
- K-mesh used for band structure and density of state$\rightarrow 12 \times 12 \times 10$
- K-mesh used for optical properties$\rightarrow 20 \times 20 \times 20$
- Convergence criteria: Energy $\rightarrow 10^{-8}$ Hartree and charge convergence $\rightarrow 10^{-6}$ electronic charge

Crystal Structure

Pb_2CoOsO_6

Crystal Information:

- Space group- 14 (*P121/c1* $\rightarrow$ monoclinic)
- Lattice parameters:
  a = 5.6365 *Å*; b = 5.5836 *Å*;
  c = 7.82833 *Å*
- Angles:
  β = 89.815°; α = γ =90°
- By replacing Co by Ni from Pb_2CoOsO_6, Pb_2NiOsO_6 is formed.

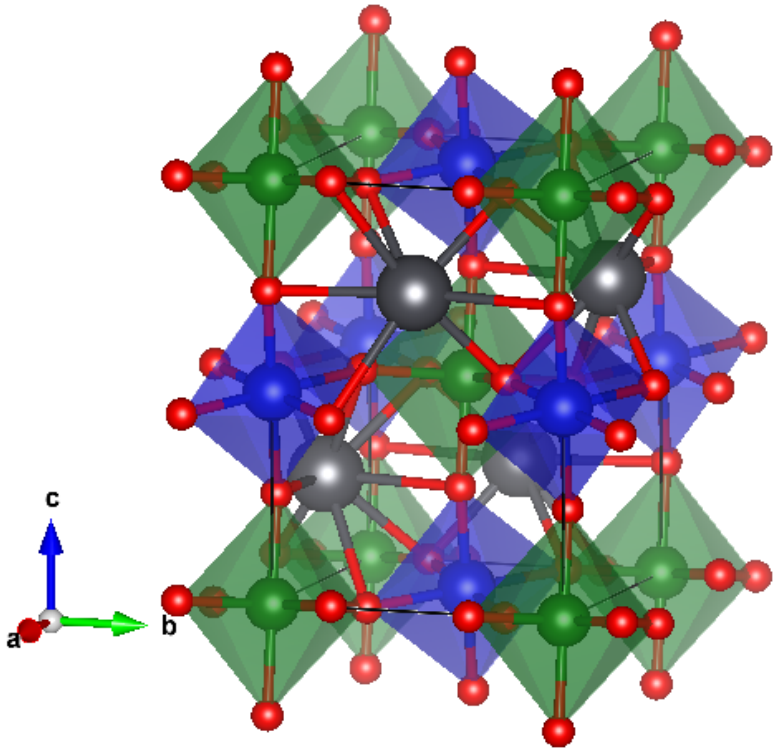

Fig: Crystal structure of Pb_2XOsO_6 (X= Co, Ni). Here green octahedra are due to XO_6 and blue octahedra are due to OsO_6 .

Results and Discussion

Ground State and Magnetic Moment

- Performed energy calculation for different magnetic configurations: one ferromagnetic state (FM-↑↑↑↑) two antiferromagnetic states (AF1-↑↓↑↓, AF2-↑↓↓↑), two ferrimagnetic states (FI1-↑↑↓↓, FI2-↑↑↑↓), and non-magnetic state.
- Pb_2CoOsO_6 has antiferromagnetic (AF2-↑↓↓↑) ground state.
- Pb_2NiOsO_6 has ferrimagnetic (FI1-↑↑↓↓) ground state.

Table: Magnetic moment of Pb_2CoOsO_6

Atoms	GGA (μ_B)	GGA+U (μ_B)
Co	2.68	3.00
Os	0.84	1.63
Total	0.00	0.00

Table: Magnetic moment of Pb_2NiOsO_6

Atoms	GGA (μ_B)	GGA+U (μ_B)
Ni	1.47	1.96
Os	1.32	1.69
Total	0.01	0.00

Results and Discussion

Density of State

- Pb_2CoOsO_6 is metal and Pb_2NiOsO_6 is half metal.
- No contribution of Co and Ni around Fermi level.
- Strong hybridization between Os-5*d* and O-2*p*near the Fermi level.

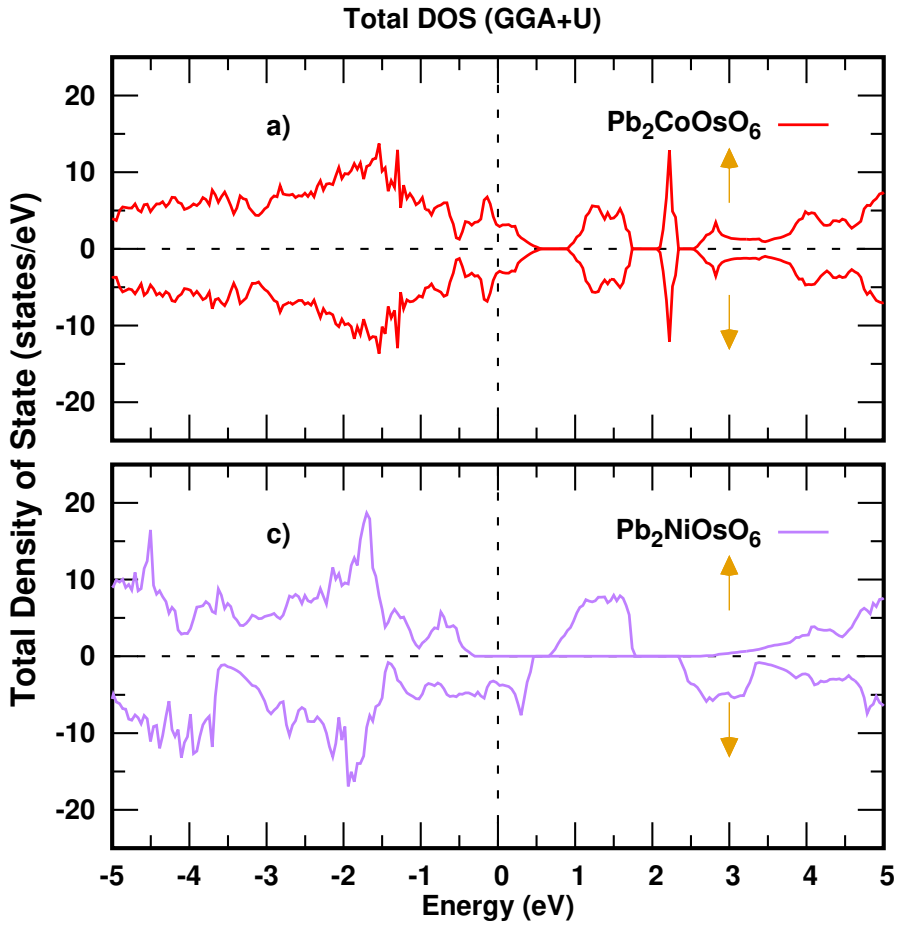

Fig: Total density of state of (a) Pb_2CoOsO_6 (b) Pb_2NiOsO_6 within GGA+*U*.

Results and Discussion

Partial density of State

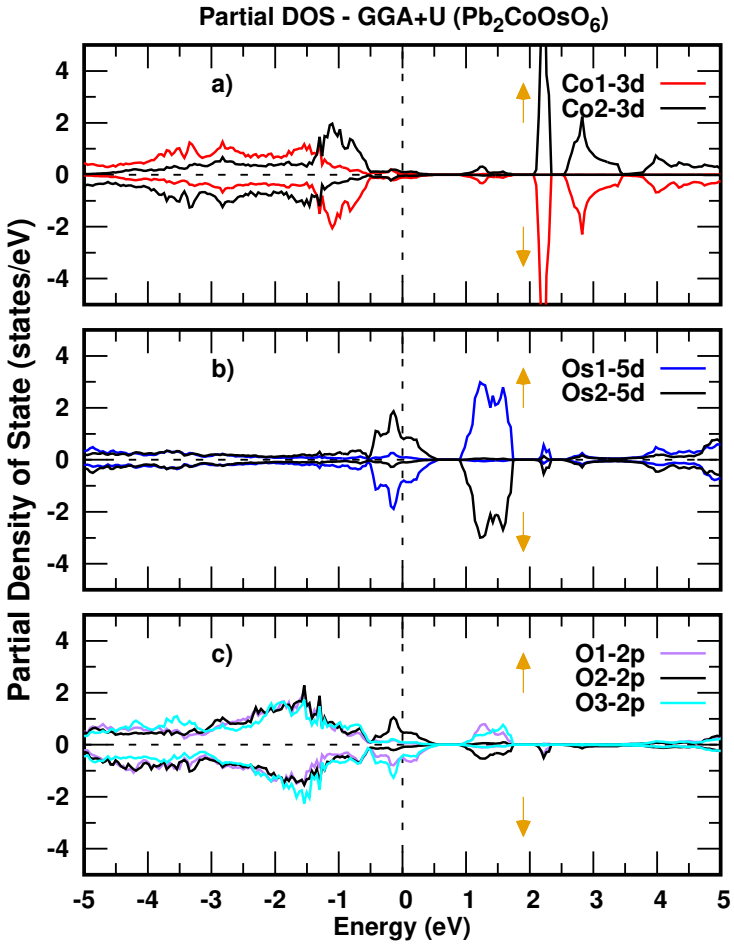

Fig: Partial density of state of Pb_2CoOsO_6 within GGA+U.

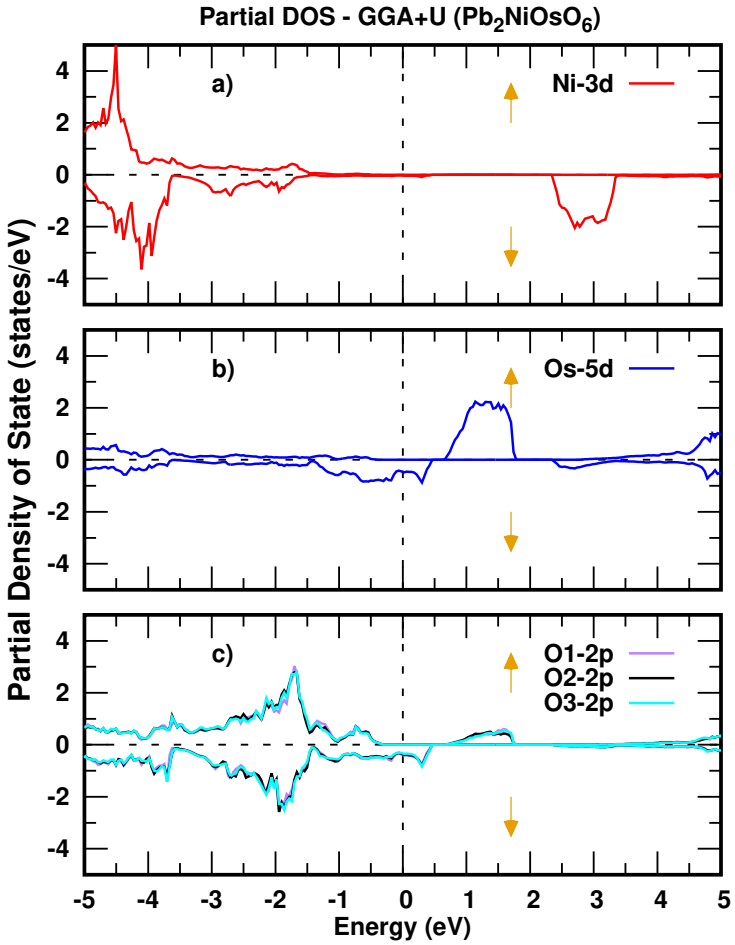

Fig: Partial density of state of Pb_2NiOsO_6 within GGA+U.

Results and Discussion

Band Structures

- Metallic nature in Pb_2CoOsO_6 and half-metallic nature in Pb_2NiOsO_6.

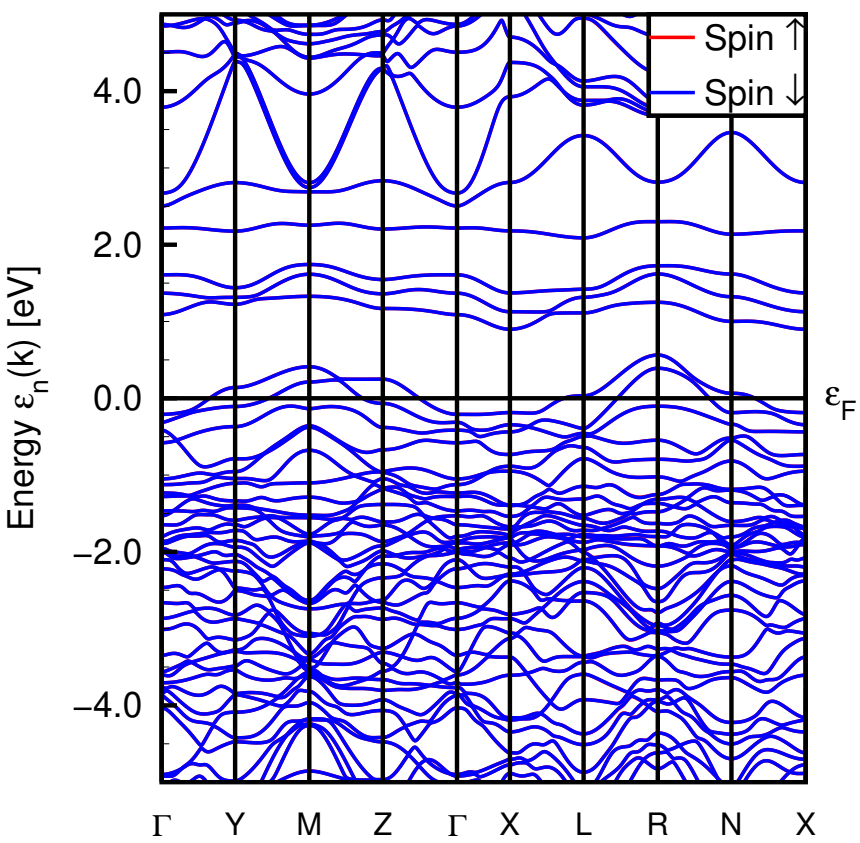

Fig: Band structures of Pb_2CoOsO_6 within GGA+U.

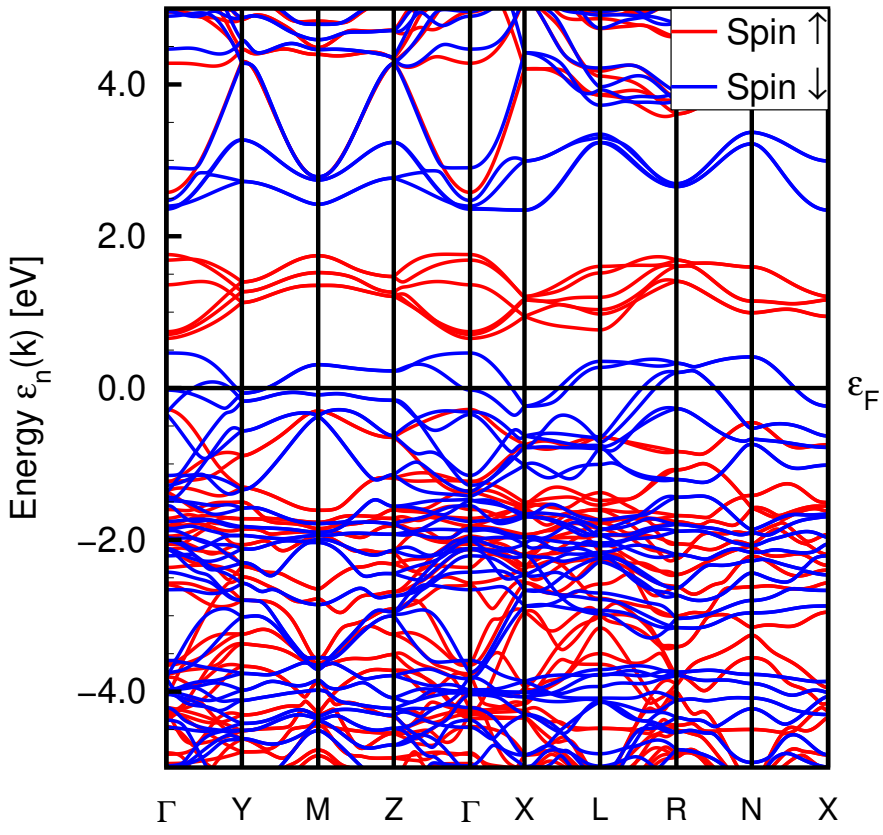

Fig: Band structures of Pb_2NiOsO_6 within GGA+U.

Results and Discussion

Optical Properties

Pb_2CoOsO_6

- Optically active in the energy range $\rightarrow$ 0 - 6.4 eV
- Significant intraband transition

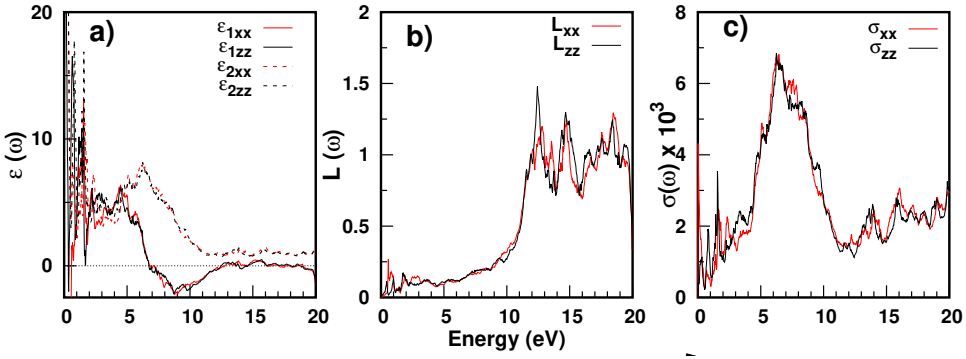

Fig: a) real (ε_1) and imaginary (ε_2) part of dielectric function, b) Loss function c) optical conductivity ($ohm^{-1}cm^{-1}$) of Pb_2CoOsO_6 within GGA+U.

Pb_2NiOsO_6

- Optically active in the energy range $\rightarrow$ 1.4 eV - 6.8 eV.

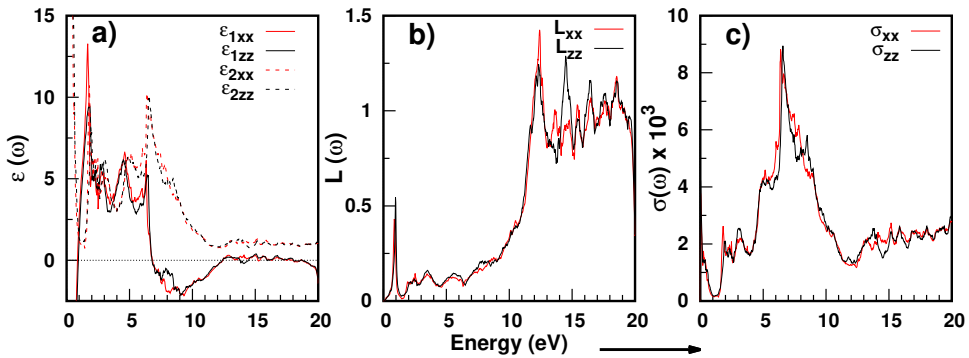

Fig: a) real (ε_1) and imaginary (ε_2) part of dielectric function, b) Loss function c) optical conductivity ($ohm^{-1}cm^{-1}$) of Pb_2NiOsO_6 within GGA+U.

Conclusions

- Pb_2CoOsO_6 is antiferromagnetic metal whereas Pb_2NiOsO_6 is ferrimagnetic half-metal.
- With electron doping in Pb_2CoOsO_6, We found electronic and magnetic phase transition.
- We observed high intraband contribution in Pb_2CoOsO_6 as compare to Pb_2NiOsO_6
- Pb_2CoOsO_6 is optically active in infrared, visible, and lower energy range of the ultraviolet region.
- Pb_2NiOsO_6 is found to be more active in the visible region and lower energy range of the ultraviolet region.

Acknowledgments

- Condensed Matter Physics Research Center, Butwal, Rupandehi, Nepal
- Sainamaina Municipality, Nepal
- Nepal Academy of Science and Technology (NAST), Nepal
- IFW Dresden, Germany