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First Principal Study of Physical Properties of Rare Earth Based Heusler Compounds X_2RuPb (X= Sc, Y and La)

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Introduction

Heusler compounds are a class of ternary intermetallics, including full Heusler X_2YZ with L_2 structure, Inverse Heusler with XA structure and Half Heusler XYZ with C1b structure. The remarkable material class comprises a vast collection of more than 1000 compounds with interesting properties and applications in spintronics, quantum information and many other fields. In this work we study the structural, elastic and electronic properties of rare earth based Heusler compounds X_2RuPb while X= Sc, Y and La.

Computational details:

in this work we perform first-principle calculation based onthe full-potential linearized augmented plane wave (FP- LAPW) method within the density functional theory (DFT)implemented in the package WIEN2K[28]. The exchange and correlation potential is treated using the generalized gradient approximation (GGA) of Perdrew-Burke- Ernzerhof [28].

Results

Structural properties:

To investigate the structural properties, we proceed a total energy minimization. The obtained structural properties are regrouped in tab1.The procedure shows that the three compounds are more stable in the full Heusler structure thanin Inverse Heusler structure. However, the Inverse Heusler type structure still holds more interesting physical propertiesand the negative calculated value of the formation energy shows that the three compounds are still mechanically stablein the Inverse Heusler type structure.

Elastic properties:

The elastic properties describe the response of a material tomacroscopic applied stress. This response gives information about the elasticity matrix which is described in cubic systems by only three constants: C11, C12 and C44. We elastic constants Cij , shear modulus G, Young modulus E, poisson ratio v, Zener anisotropic factor A and Pugh ratio B/G in both structure types.

Electronic properties:

To investigate the electronic nature of our inverse Heusler compounds, we present the band structure at the theoreticalequilibrium lattice constant along the high symmetry directions of the first Brillouin zone. The calculation showsthat the band structure of Y_2RuPb has a direct band gap of 0.058 eV at Γ point while the band structures of Sc_2RuPb and La_2RuPb have indirect band gaps of 0.193 eV and 0.164 eV respectively which is in good agreement with previous calculations.

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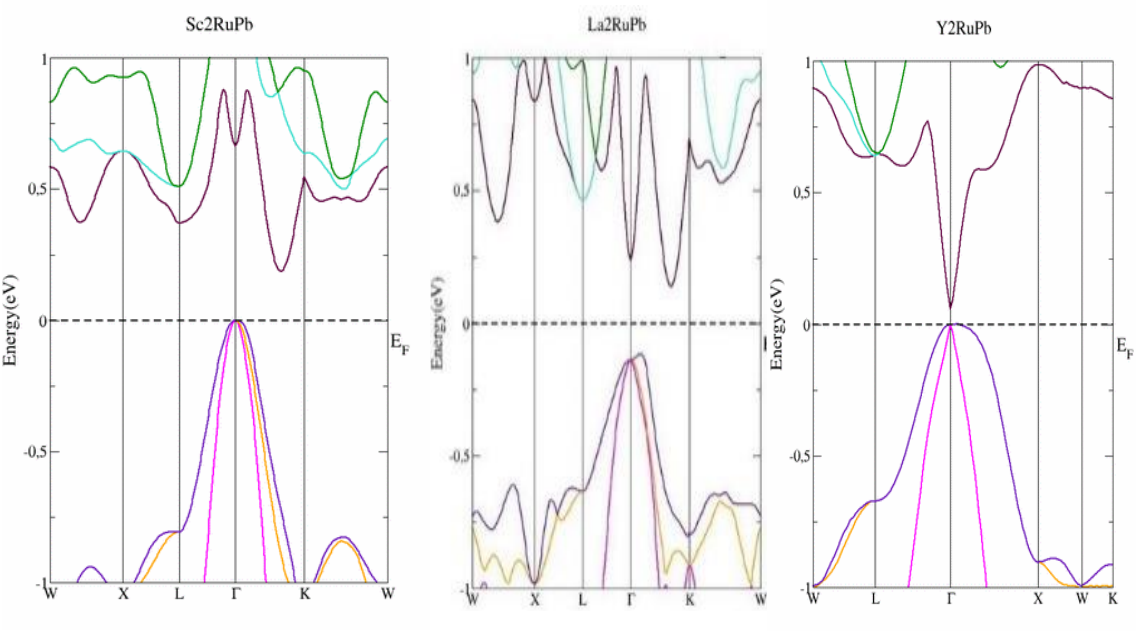

Fig 1: Band structure of Sc_2RuPb, Y_2RuPb and La_2RuPb

Table1: calculated lattice parameters a0, corresponding total energies and Bulk modulus for Sc_2RuPb, Y_2RuPb and La_2RuPb in both regular and inverse structure types.
a: [3]
b: [4]

compound		Sc_2RuPb		Y_2RuPb		La_2RuPb	
Structure type		Regular Heusler	Inverse Heusler	Regular Heusler	Inverse Heusler	Regular Heusler	Inverse Heusler
a_0 (Å)	Our cal. other	6.8405 6.835[a]	6.7531 6.746[a] 6.670[b]	7.2496 7.245[a]	7.0871 7.082[a] 7.085[b]	7.6219 7.630[a]	7.3417 7.376[a] 7.347[b]
Total Energy (Ry)	Our cal. other	-53978.045 -53978.066[a]	-53978.026 -53939.810[b]	-64463.975 -64463.992[a]	-64463.935 -64463.952[a]	-84911.727 -84911.736[a]	-84911.720 -84911.718[a]
Bulk modulus (GPa)	Our cal. other	101.96 101.688[a]	106.74 106.221[a]	83.393 82.519[a]	87.461 85.647[a]	65.422 67.475[a]	76.003 77.435[a]

Conclusion

the study of structural and elastic properties has shown that the compounds Sc_2RuPb, Y_2RuPb and La_2RuPb stabilize in both full and inverse heusler type structures. However, the inverse heusler type is more suitable to hold interesting electronic properties. The band structure of the three compounds in inverse heusler type shows a semiconductor behavior that can be useful in thermoelectricity and radiation semiconductor detectors.

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