

# ADVANCES IN CONTEMPORARY PHYSICS

HIGH-ENERGY, COSMOLOGY,  
AND SOFT MATTER



Dr. Syed Salman Ahmad Warsi

# **Advances In Contemporary Physics**

**High-Energy, Cosmology, and Soft Matter**

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# COMPARATIVE ANALYSIS OF STRUCTURAL, ELECTRONIC AND THERMAL PROPERTIES OF AIRE (RE = Y, Pr, Gd)

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The properties of AIRE in B2 structure have been analysed using the first-principles method. The structural and electronic properties were investigated using the generalized gradient approximation (GGA) method and by TBLMTO method in the context of density functional theory. The electronic band structure calculations carried out to obtain the total energy of the AIRE (RE= Y, Pr, Gd) inter-metallic compound using the first principles FP-LAPW method by Shugani *et al* and that using TB-LMTO method by Srivastava *et al* have been compared with experimental data. The equilibrium cell volume  $V_0$  is found to be 315.90 a.u.<sup>3</sup> and 294.82 a.u.<sup>3</sup> (43.69 Å<sup>3</sup>) for AIY by FP-LAPW and TB-LMTO respectively. While  $V_0$  for AlPr and AlGd is 322.36 a.u.<sup>3</sup>, 297.58 a.u.<sup>3</sup> (44.099 Å<sup>3</sup>) and 307.57 a.u.<sup>3</sup>, 283.55 a.u.<sup>3</sup> (42.02 Å<sup>3</sup>). The computed lattice parameter (3.604 Å) and bulk modulus (62.40 GPa) by TB-LMTO and 3.522 and 79.5 for AIY by FP-LAPW method while 3.628 Å, 65.5 GPa for AlPr, 3.572 Å, 49.42 GPa for AlGd by TB-LMTO and 3.533 Å, 55.11 GPa for AlPr, 3.47 Å, 70.60 GPa for AlGd by FP-LAPW method. The electronic band structure and energy-dependent density of states reveal the metallic nature of the titled Rare-earth inter-metallic compounds.

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## INTRODUCTION:

An intermetallic, also called ordered intermetallic alloy, is a solid-state compound exhibiting metallic bonding, defined stoichiometry and ordered crystal structure. These alloys involve solid phases, which contain two or more metallic elements, with one or more non-metallic elements (optionally), whose crystal structure may be different from that of the constituent atoms. Many intermetallic compounds exhibit striking physical and mechanical properties, likewise high melting point, low density and good oxidation or corrosion resistance. This has led to their utilization in structural and non-structural applications [1, 2]. The intermetallic compounds are generally brittle or semi-brittle at room temperature, making them difficult to utilize in structural applications, such as aluminides and silicides show brittleness due to environmental effect, but can be overcome by alloying, microstructural control or coating. Examples of such compounds that are adversely affected by moist environments are FeAl, Fe<sub>3</sub>Al, Ni<sub>3</sub>Al and Ni<sub>3</sub>Si [1]. Two important roads to improve the room temperature ductility have been used: the alloying with