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# First-principles calculations on the electronic structure and thermoelectric properties of quaternary Heusler compounds: LiScPtSi and LiScPdGe

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ABSTRACT

This research work explores the two quaternary Heusler compounds within the 18-valence electron formalism i.e. LiScPtSi and LiScPdGe as the capable thermoelectric materials in the temperature range of 1200 K. The band structure of these compounds reports the indirect bandgap of 1.08 eV for LiScPtSi and 0.5352 eV for LiScPdGe, also declares as p-type semiconductors. This report presents the structural, electronic, phonon, elastic and mechanical properties for the practical utilization of the materials. The melting point of LiScPtSi and LiScPdGe are calculated as 1561 ± 300 K and 1245 ± 300 K respectively; owing to this fact all the prime thermoelectric properties along with the Figure of Merit (ZT) are calculated in the temperature range of 1200 K. The investigated materials are purely anisotropic with ductile property (can be stretched as wires), dynamically and mechanically stable. In an overview of thermoelectric properties, the Seebeck coefficient and the lattice thermal conductivity at 300 K for LiScPtSi are 1784 μV/K, 39.6 W/mK and for LiScPdGe are 894μV/K, 27.7 W/mK respectively. Nevertheless, the respective maximum Figure of Merit (ZT) is 0.57 and 0.53 at the 1200 K that ensures the materials to be efficient thermoelectric elements in the high-temperature range with reliable material properties. As the materials are first time investigated here in the detailed prospectus; the proposed research work is proficient to be considered in experimental research as well as for energy conversion applications.

## 1. Introduction

The world population and ultra-modern lifestyle enhance the energy consumption, which in turn demands the availability of safe and pollution-free energy resources in all scales and regions. Due to this, in the world of the energy crisis, researchers hunt for novel and convenient methods to improve energy conversion techniques. However, the traditional energy resources are efficient but due to pollution and radiation accidents, they can't be considered as reliable future energy assets. At this moment 'Thermoelectricity' is one of the prerequisite kinds of anticipation that is reliable for the direct conversion of heat into electric energy [1,2]. The materials holding this technology (thermoelectricity) are known as thermoelectric materials; was introduced by Thomson Johann Seebeck in 1821. The thermoelectric materials generate the Thermo e.m.f within the temperature gradient; hence, this is a platform where the waste heat energy can be utilized by its conversion into electric energy. In Thermo Electric Modules (TEM) there is no use of any toxic material, no complex designing and no use of any kind of fuels. Due to all such merits, this technique has been announced as the 'Green Technology' of energy generation [3]. This is another important feature that the thermoelectric modules (TEM) don't require any kind of produced heat (like of the thermal power plants) but they can be easily installed anywhere and everywhere in the wasted heat regions to utilize the available waste heat. Due to this they have become

*Abbreviations:* TEM, Thermo Electric Modules; DFT, Density Functional Theory; ZT, Thermoelectric Figure of Merit.

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