

7.	<b>No. of paper Published:</b> UGC Care list Journals=12 Non UGC care list Journal Citations	i. 5 points per paper ii. 2 points per paper iii. 1 point per 20 citations	20/20
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**Prof. Prakash Chand**, AP Public Administration has published two research papers in UGCCare list journals.

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**Prof. Vidhu Bhardwaj**, Department of English has published one research paper in an International peer reviewed Journal and one research paper in National peer reviewed Journal.

**Dr. Smriti**, AP Zoology has published two research papers in UGC Care list journals.

**Dr. Kuldeep AP Commerce** has published 2 paper in UGC Care and 2 in Non UGC Care listed Journals.

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**Effects of metals (X = Pd, Ag, Cd) on structural, electronic, mechanical, thermoelectric and hydrogen storage properties of LiXH<sub>3</sub> perovskites**  
 Anupam <sup>a</sup>, Shyam Lal Gupta <sup>b</sup>, Sumit Kumar <sup>c</sup>, Sanjeev Singh Thakur <sup>d</sup>, Ashwani Kumar <sup>e</sup>, Sanjay Parwar <sup>f</sup>, Divaker <sup>g,\*</sup>

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**Keywords:**  
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 Li metal hydrides  
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**ABSTRACT**  
 Using the WIEN2K code, the hydrogen storage capabilities of lithium compositions like LiXH<sub>3</sub> (X = Pd, Ag, Cd) hydrides are examined. Structural, electronic, mechanical, thermoelectric, and hydrogen storage parameters of these hydrides are analyzed using first-principles simulations. Structural analysis of these compositions reveals that the hydrides are stable and belong to the cubic space group number (221 Pm-3 m). The thermodynamic stability of these hydrides are given in terms of formation energies and stability is checked through phonon dispersion curves. The purpose of the study is to calculate formation energy and breakdown temperature to determine stability of these hydrides. The metallic nature of all compositions are confirmed by band plots and density of states. The elastic properties are calculated to check the applicability of these compositions for applications involving hydrogen storage. The present paper expresses the initial theoretical approach towards the future exploration of these materials for hydrogen storage applications.

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**1. Introduction**

Energy crisis are a result of the rising demand for fossil fuels like coal, oil, and petroleum. Combusting fossil fuels causes the release of dangerous toxic gases like chlorofluorocarbon (CFC), CO<sub>2</sub>, N<sub>2</sub>O, CH<sub>4</sub>, and others that harm the environment. As a result, it is challenging for researchers around the world to look into other alternative sources of energy [1–5]. Since hydrogen is a clean, non-toxic, and renewable source of energy, it is used as a substitute for existing non-renewable energy sources to fulfill the need for energy. Hydrogen is abundant in nature and can be used for a variety of purposes, including cooking, electricity production, running factories and even planes, the automobile industry, and supplying domestic energy needs. With hydrogen-powered cars, the automobile industry has a lot of potential in the transportation sector. Significant obstacles exist for both the extraction and storage of hydrogen [10–20]. Its storage density needs to be increased to make it commercially feasible. For the storage of hydrogen at high density, several techniques have been developed, including cryogenic form, compound form, and pressurized gas form. The second method for storing hydrogen is the most promising, aspirational, and

developing. The storage of hydrogen in solids is preferred over that of liquid and pressurized gas. Metal organic frameworks and carbon nanotube can store hydrogen using the chemisorption or physisorption processes. The high volumetric density of hydrogen atoms in the host lattice makes metal hydrides suitable for hydrogen storage applications as well. Favorable thermodynamic characteristics and structural stability of metal hydrides are additional factors that make them appropriate for applications involving hydrogen storage [21]. Researchers are currently facing a significant challenge in fully comprehending the kinds of materials that can deposit large amounts of hydrogen as fuel [22,23]. In our efforts towards that we have recently studied Zirconium based ZrX<sub>3</sub> (X = Zn, Cd) hydride perovskites and found them to be reasonable importance for hydrogen storage applications [1]. In continuation to that we are now presenting another study on Li based compositions LiXH<sub>3</sub> (X = Pd, Ag, Cd) perovskite as potential candidates for hydrogen storage materials although many lithium based hydrides are studied earlier as well using DFT [24–27]. Our proposed compositions are yet not explored and found to be a potential candidate for hydrogen storage applications. We have explored the structural, mechanical, electronic,

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Spin-polarized DFT investigations of novel KV5B half-Heusler compound for spintronic and thermodynamic applications

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ARTICLE INFO

Keywords: Spintronics, DFT, Magnetic moments, Thermodynamic properties, Thermoelectric properties

ABSTRACT

In this study we have investigated the robust phase stability, elastic mechanical, thermophysical and magnetic properties of KV5B half Heusler compound by implementing density functional theory (DFT) module in VESTA simulation package. The dynamic phase stability is confirmed by phonon dispersion curves...

1. Introduction

In the recent years, researchers around the globe have revealed remarkable interest in spintronic materials owing to their wide range of functionality in various domains [1-3]. Spintronics is a rapidly expanding field which comes into view on regulating the electron intrinsic spin properties to achieve the high speed information processing and large storage [4].

storing information [5-7]. Heusler compounds exhibit spin dependent electronic properties which is generally known as half metallic behavior where the materials show metallic nature for one spin (up or down) electrons and non-conducting for the other (down or up) electron simultaneously [8,9].

Thermoelectricity (TE) is a technology known for the thermoelectric effect which convert heat into electric current and vice-versa without involving the movement. It is one of robust source of clean energy. Thermoelectric technology may be incorporated to create the waste heat recovery from automobiles, refineries, other industrial plants and significantly contribute to the objectives in achieving zero carbon emission.

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A newly proposed full Heusler alloy Ir2VZ (Z = Sn, In) suitable for high-temperature thermoelectric applications: A DFT approach

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We calculated the structural, electronic, mechanical and thermoelectric properties of the Ir2VZ-based, newly proposed Heusler alloys Ir2V (In, Sn). Both alloys have an indirect

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Ab initio studies of newly proposed zirconium based novel combinations of hydride perovskites ZrXH3 (X = Zn, Cd) as hydrogen storage applications

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ARTICLE INFO

Keywords: Density functional theory, Electronic structure, Hydrogen storage, Perovskites, Hydrides

ABSTRACT

Using the VESTA code, first-principles simulations of ZrXH3 (X = Zn, Cd) hydride perovskites are performed to determine their hydrogen storage properties. The purpose of this study is to investigate their structural, optoelectronic, hydrogen storage, mechanical and thermoelectric properties. The structural analysis demonstrates their stability through the heat of formation along with desorption temperature and shows that these compositions belong to the orthorhombic space group Cmcm (no. 63). The band structure and density of states are estimated for electronic characteristics, indicating the metallic nature of both compositions. Analysis of elastic properties such as elastic constants, Pugh's ratio, bulk modulus, Poisson's ratio, and anisotropy factor are explored to determine the mechanical stability of these compositions and demonstrate their suitability as a transport medium in hydrogen storage systems even at higher pressure. To study the optical behavior of the perovskites under consideration for hydrogen storage application, the dielectric parameters, dielectric constants, refractive index, optical conductivity, absorptionity, and energy loss function are studied. The present paper represents the initial theoretical effort toward future exploration of these materials for hydrogen storage application.

1. Introduction

The demand for clean and efficient energy sources has attracted extensive research efforts of researchers in the field of hydrogen storage materials. Hydrogen, as a clean and versatile energy carrier, has emerged as a promising alternative to fossil fuels, offering potential solutions to mitigate the environmental impact of energy production and consumption [1-11]. However, the efficient storage of hydrogen remains a significant challenge due to its low density and the requirement for safe and practical storage methods. Efficient hydrogen storage materials play a pivotal role in the development and practical implementation of hydrogen-based energy systems [12-24]. Among various materials, metal hydrides, particularly perovskite compositions, have garnered significant attention due to their favorable hydrogen storage properties, such as high storage capacity, reversibility, stability, their unique structural properties and versatile chemical compositions [25-30]. These materials are represented by the general formula ABX3, possess an orthorhombic structure at ambient conditions. The intrinsic flexibility of perovskite structures allows the incorporation of various elements, making them attractive candidates for development of new

hydrogen storage materials [31-33]. These materials possess an intriguing combination of properties, including desirable thermodynamic stability, low density, and suitable hydrogen adsorption/desorption kinetics. However, the detailed understanding of the underlying atomic and electronic structures, as well as the thermodynamic and kinetic properties governing the hydrogen storage behavior in Zr based perovskites, remains largely unexplored. As density functional theory (DFT) based first principles investigations provide an efficient approach to elucidate the structural, electronic, and other properties of materials [34,35], enabling us to comprehend their fundamental behavior at the atomic scale therefore to bridge this knowledge gap, we propose to investigate new Zr based compositions ZrXH3 (X = Zn, Cd) perovskite materials for hydrogen storage applications. The primary objectives of this work are focused on (1) to computationally evaluate the thermodynamic stability of ZrXH3 (X = Zn, Cd) perovskites as potential hydrogen storage materials; (2) to investigate underlying mechanisms responsible for hydrogen adsorption and desorption in these materials; and (3) to elucidate the effects of chemical substitution (X = Zn, Cd) on the hydrogen storage properties of Zr-based perovskites. Through a

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**Spin-polarized DFT investigations of novel KV5b half-Heusler compound for spintronic and thermodynamic applications**

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**ARTICLE INFO**      **ABSTRACT**

**Keywords:**  
 Spintronic  
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In this study we have investigated the robust phase stability, elasto-mechanical, thermophysical and magnetic response of KV5b half-Heusler compound by implementing density functional theory (DFT) within a WIEN2k simulation package. The dynamic phase stability is computed in phase type I, II & III phase configurations by optimizing their energy. It is observed that given compound is more stable in spin-polarized state of phase type-II. To explore the electronic band structure, we apply the generalized gradient approximation along with Hubbard potential U. The electronic band profile of the Heusler alloy display a half-metallic nature. Moreover, the calculated second-order elastic parameters divulge the brittle nature. To understand the thermodynamical and thermoelectric stability of the alloy at various temperature and pressures range Quasi-Harmonic Debye model is executed successfully. The computed value of magnetic moment (MM) found in good agreement with Slater-Pauling rule. Our findings confirm that the predicted half Heusler alloy can be used in various spintronic and thermoelectric applications.

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**INTERNATIONAL JOURNAL OF CREATIVE RESEARCH THOUGHTS (IJCRT)**  
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**Digitalization And Their Impact On Perception Of Investor In Stock Market -Age-Wise Analysis**

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**Abstract:**  
 Digitalization of stock market is one phenomenon of investment and there multiple effects have been observed in investor perception in recent past. It also give an access to the digitalization of stock market. This research work is partly and primarily seeking anticipation. While making perception of stock market digitalization of stock market in the present paper focusing the independent variables which are of several types. Both new study which are related the perception of investor after digitalization of stock market. The literature related this paper is in period of digitalization. This research work is also change in the working of stock market also witness in recent past and also resulting in reduce a perception in digital world. In order to get familiar with this research, researcher the present study consideration and also to know the extent of digitalization has an impact on safety, security, reliability and others aspects with the change in technology.

**Keywords:** Digitalization, Investors working, Transaction and Security

**Introduction:**  
 Financial markets especially stock market is experiencing challenges in the recent years due to changes in national and international level which has changed the working of stock market. Emerging aspects of these changes in Digitalization of stock market. Digitalization has changed working aspects of stock market. In order to know in what extent digitalization has an impact on safety, security, reliability and others aspects, with the change in technology the present paper throws light on the basis of selected demographic variables. The present technology in stock market is digitalization. Machine Learning and Data Analytics playing a pivotal role in investment in stock market. The entry of these technologies provides a wide range of investment options to stock market. The entry of these technologies provides a general idea on safety, security, reliability and others aspects with the change in technology.

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