<u>7.</u>	**No. of paper Published:** 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**

Prof. Prakash Chand, AP Public Administration has published two research papers in UGCCare list journals.

Prof UpmaDhiman, Associate Professors Commerce has published two research papers in UGC Care list journals.

Prof. Vidhu Bhardwaj, Department of Englishhas published one research paper in an Internationalpeer 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.

A.P. Anupam AP Physics has published six research papers in UGC Care list journals.

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Effects of metals (X = Pd, Ag, Cd) on structural, electronic, mechanical, thermoelectric and hydrogen storage properties of $LiXH_3$ perovskites

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Keywords:
Electronic capacity
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Goldschmidt factor (t)
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Thermodynamic stability

ABSTRACT

Using the WIEN2K code, the hydrogen storage capabilities of lithium compositions like $LiXH_3$ (X = Pd, Ag, Cd) hydrides are examined. Structural, electronic, mechanical, thermoelectric, and hydrogen storage properties 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 represents the initial theoretical approach towards the future exploration of these materials for hydrogen storage applications.

1. Introduction

Energy crises are a result of the rising demand for fossil fuels like coal, oil, and petroleum. Consuming fossil fuels causes the release of dangerous toxic gases like chlorofluorocarbon (CFC), CO_2, N_2O, CH_4, 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 [1–9]. 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 aero 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 $ZrXH_3$ (X = Zn, Cd) hydride perovskites and found them to be of reasonable importance for hydrogen storage applications [1]. In continuation to that we are now presenting another study on Li based compositions $LiXH_3$ (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 projected 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 KVSb half-Heusler compound for spintronic and thermodynamic applications

Ashwani Kumar, Shyam Lal Gupta, Vipan Kumar, Sumit Kumar, Anupam, Diwaker*

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ABSTRACT

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A newly proposed full Heusler alloy $Ir_2VZ(Z = Sn, In)$ suitable for high-temperature thermoelectric applications: A DFT approach

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We calculated the structural, electronic, mechanical and thermoelectric properties of the iridium-based, newly proposed Heusler alloys Ir_2V (In, Sn). Both alloys have an indirect

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Ab initio studies of newly proposed zirconium based novel combinations of hydride perovskites $ZrXH_3$ (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 WIEN2k code, first-principles simulations of $ZrXH_3$ (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 applications, the dielectric parameters, dielectric constants, refractive index, optical conductivity, absorptivity, and energy loss function are studied. The present paper represents the initial theoretical effort toward future exploration of these materials for hydrogen storage applications.

1. Introduction

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

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ARTICLE INFO

Keywords:
Spintronics
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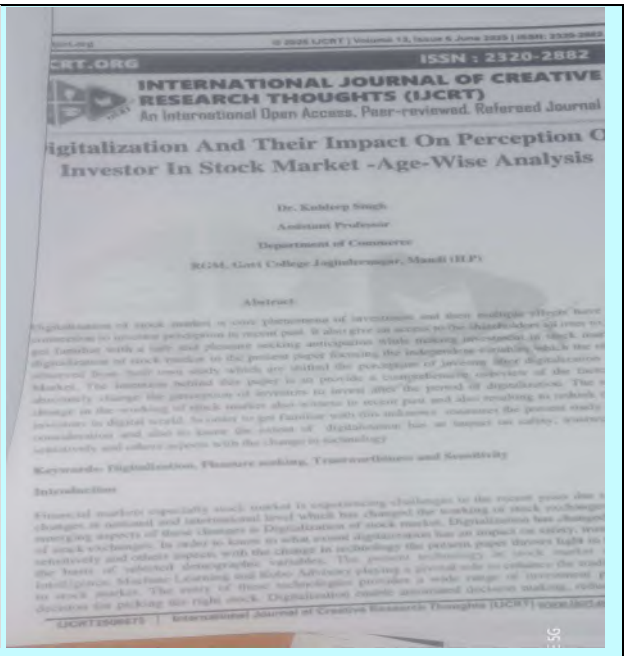
Magnetic moments
Thermodynamic response
Thermoelectric properties

ABSTRACT

In this study we have investigated the robust phase stability, elasto-mechanical, thermophysical and magnetic response of KVSb half Heusler compound by implementing density functional theory (DFT) models in WIEN2k simulation package. The dynamic phase stability is computed in phase type I, II & III phase configurations by optimising their energy. It is observed that given compound is more stable in spin-polarized state of phase type-III. To explore the electronic band structure, we apply the generalised 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 ranges Quasi-Harmonic Debye model is executed successfully. The computed value of magnetic moment (MM) found in good agreement with Slater-Pauling rule. Our findings confirms that the predicted half Heusler alloy can be used in various spintronics and thermoelectric applications.



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A newly proposed full Heusler alloy $Ir_2VZ(Z = Sn, In)$ suitable for high-temperature thermoelectric applications: A DFT approach [PDF] re

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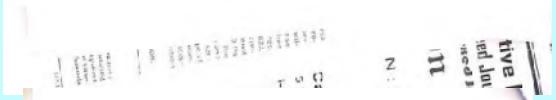

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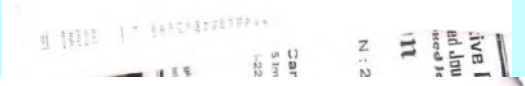

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... to investigate new Zr based compositions **ZrXH 3** (X = Z Cd) ... evaluate the thermodynamic stability of **ZrXH 3** (X = Zn, Cd) ... into the hydrogen storage behavior of **ZrXH 3** (X Zn, Cd) ...

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