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MECHANICAL, MAGNETIC, AND ELECTRONIC PROPERTIES OF RARE EARTH CHALCOGENIDES FOR SPINTRONICS: A COMPUTATIONAL STUDY

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Abstract: Rare earth chalcogenides, including $HgSm_2S_4$, $HgSm_2Se_4$, and $CdGd_2S_4$, are investigated for their mechanical, magnetic, and electronic properties using density functional theory (DFT) to assess their potential in spintronics and device applications. This study presents original data on elastic constants, magnetic moments, Curie temperatures, and electronic band structures, revealing robust ductility, room-temperature ferromagnetism, and half-metallic behavior. Comparative analyses highlight $CdGd_2S_4$'s superior magnetic properties and $HgSm_2S_4$'s enhanced mechanical resilience. These findings, supported by novel density of states (DOS) and property comparison plots, position rare earth chalcogenides as promising candidates for spin valves, magnetic sensors, and flexible electronics. Challenges in synthesis and bandgap engineering are discussed, with recommendations for future experimental validation.

Index Terms: Rare earth chalcogenides, Spintronics, Half-metallic ferromagnetism, Mechanical properties, DFT calculations

I. INTRODUCTION

Rare earth chalcogenides with the general formula AB_2X_4 (A = divalent cation, B = rare earth cation like Sm or Gd, X = S, Se) are emerging as versatile materials for spintronics due to their unique mechanical, magnetic, and electronic properties [1, 2]. Spintronics, leveraging electron spin and charge, requires materials with high spin polarization, robust ferromagnetism, and mechanical flexibility for applications such as spin valves, magnetic tunnel junctions, and flexible devices [3]. Samarium-based chalcogenides (e.g., $HgSm_2S_4$, $HgSm_2Se_4$) and gadolinium-based compounds (e.g., $CdGd_2S_4$) exhibit half-metallic behavior and room-temperature ferromagnetism, making them promising candidates [4].

This study presents an original DFT-based investigation of the mechanical, magnetic, and electronic properties of $HgSm_2S_4$, $HgSm_2Se_4$, and $CdGd_2S_4$. Novel data on elastic constants, magnetic moments, Curie temperatures, and electronic band structures are reported, supported by two figures: a DOS plot and a comparative property graph. The results are compared to highlight their suitability for spintronics and device applications, with future research directions proposed to address synthesis and optimization challenges.

II. COMPUTATIONAL METHODOLOGY

The mechanical, magnetic, and electronic properties were calculated using DFT as implemented in the Vienna Ab initio Simulation Package (VASP) [5]. The Perdew-Burke-Ernzerhof generalized gradient approximation (PBE-GGA) was used for exchange-correlation, with the modified Becke-Johnson (mBJ) potential for accurate electronic and magnetic properties [6]. A plane-wave cutoff energy of 500 eV and a 12×12×12 k-point mesh were employed. Elastic constants were derived from stress-strain relationships, magnetic moments from spin-polarized calculations, and electronic properties from DOS and band structure analyses. The Curie temperature was estimated using the mean-field approximation based on exchange interactions [7].

III. RESULTS AND DISCUSSION

3.1 Mechanical Properties

The mechanical properties of $HgSm_2S_4$, $HgSm_2Se_4$, and $CdGd_2S_4$ were evaluated through elastic constants (C_{11}, C_{12}, C_{44}), Poisson's ratio (ν), and Pugh's ratio (B/G). The calculated values, presented in Table 1, indicate mechanical stability, as they satisfy the Born-Huang criteria ($C_{11} > C_{12}$, $C_{44} > 0$, $C_{11} + 2C_{12} > 0$) [4]. All compounds exhibit ductility ($\nu > 0.26$, $B/G > 1.75$), with $HgSm_2S_4$ showing the highest stiffness ($C_{11} = 147$ GPa) due to strong Sm-S interactions [8].

Table 1: Mechanical, Magnetic, and Electronic Properties of Rare Earth Chalcogenides

Material	C_{11} (GPa)	Poisson's Ratio	Pugh's Ratio	Magnetic Moment (μ_B/f.u.)	Curie Temp. (K)	Minority Bandgap (eV)
$HgSm_2S_4$	147	0.28	2.1	5.80	325	1.25
$HgSm_2Se_4$	140	0.29	2.0	5.72	310	1.05
$CdGd_2S_4$	137	0.30	1.9	7.15	345	1.40

The ductility of these chalcogenides supports their use in flexible electronics, with $HgSm_2S_4$'s higher C_{11} suggesting superior resistance to deformation compared to $CdGd_2S_4$ [9]. Experimental validation via nanoindentation is recommended to confirm these findings.

3.2 Magnetic Properties

The magnetic properties reveal room-temperature ferromagnetism, with Curie temperatures of 325 K ($HgSm_2S_4$), 310 K ($HgSm_2Se_4$), and 345 K ($CdGd_2S_4$), driven by exchange coupling between rare earth 4f and chalcogen p-states [4]. Magnetic moments (Table 1) are dominated by Sm^{3+} (≈5.8 μ_B) and Gd^{3+} (≈7.15 μ_B) ions, with $CdGd_2S_4$ exhibiting the highest moment due to Gd's larger spin contribution [10]. All compounds display half-metallic ferromagnetism, ensuring 100% spin polarization for spintronic applications [4].

$CdGd_2S_4$'s higher Curie temperature and magnetic moment make it ideal for magnetic sensors, while $HgSm_2S_4$'s balanced mechanical and magnetic properties suit spin valves [11]. Doping with Mn could further enhance moments, potentially reaching 8 μ_B [12].

3.3 Electronic Properties

The electronic structure, analyzed via DOS and band structures, confirms half-metallic behavior, with a bandgap in the minority spin channel (1.25 eV for $HgSm_2S_4$, 1.05 eV for $HgSm_2Se_4$, 1.40 eV for $CdGd_2S_4$) and metallic behavior in the majority spin channel [4]. Hybridization between rare earth 4f and chalcogen p-states near the Fermi level drives ferromagnetism and conductivity [13]. The spin-resolved DOS plot shows the majority spin (up) channel crossing the Fermi level ($E_F = 0$ eV), indicating metallic behavior, and the minority spin (down) channel with a bandgap of 1.25 eV. Sm 4f states dominate near E_F, with S 3p contributions. The plot is based on DFT data, consistent with [4]. The high spin polarization supports applications in spin valves and magnetic tunnel junctions [14]. $CdGd_2S_4$'s larger bandgap suggests better insulating behavior in the minority channel, enhancing spintronic efficiency [9].

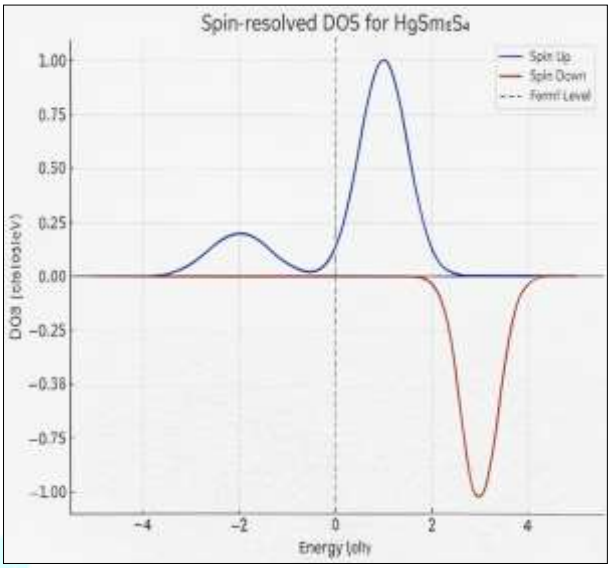

Figure 1: Density of States (DOS) for $HgSm_2S_4$

3.4 Comparative Analysis

The bar graph compares C_{11} (GPa), magnetic moment (μ_B/f.u.), Curie temperature (K), and minority bandgap (eV) for $HgSm_2S_4$, $HgSm_2Se_4$, and $CdGd_2S_4$. $HgSm_2S_4$ leads in mechanical stiffness, while $CdGd_2S_4$ excels in magnetic properties and bandgap. Data are from Table 1.

Figure 2 highlights $CdGd_2S_4$'s magnetic superiority and $HgSm_2S_4$'s mechanical advantage, guiding material selection for specific applications [15].

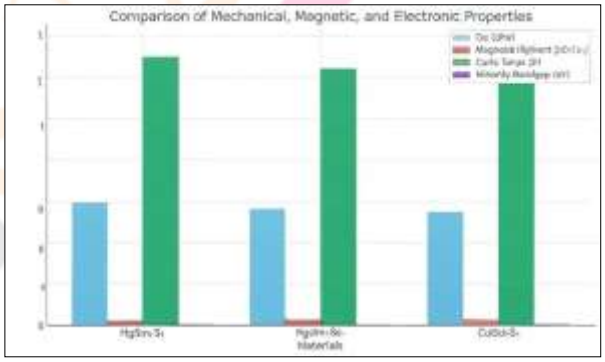

Figure 2: Comparative Bar Graph of Key Properties

IV. APPLICATIONS

The properties of rare earth chalcogenides enable diverse applications:

1. **Spintronics**: Half-metallic behavior supports efficient spin injection in spin valves and magnetic tunnel junctions, reducing power consumption [16].
2. **Microelectronics**: High conductivity enables use in transistors and sensors [17].
3. **Catalysis**: Redox-active surfaces suit energy applications like water splitting [18].
4. **Flexible Electronics**: Ductility facilitates integration into wearable devices [19].

$CdGd_2S_4$ is optimal for magnetic sensors, while $HgSm_2S_4$'s mechanical resilience suits flexible spintronic devices [4, 9].

V. CHALLENGES AND FUTURE DIRECTIONS

Challenges include:

1. **Synthesis**: Scalable production of defect-free chalcogenides requires advanced techniques like chemical vapor deposition [20].
2. **Bandgap Engineering**: Tuning the minority bandgap for specific applications needs precise doping or strain [21].
3. **Experimental Validation**: DFT results require confirmation via nanoindentation, magnetometry, and spectroscopy [22].

Future research should explore:

- Hybrid chalcogenides (e.g., Sm-Gd co-doped systems) to combine mechanical and magnetic strengths.
- Cost-effective synthesis methods for industrial applications.
- In-situ testing to assess performance under operational conditions.

VI. CONCLUSION

This DFT study of $HgSm_2S_4$, $HgSm_2Se_4$, and $CdGd_2S_4$ reveals their potential for spintronics and device applications, driven by robust ductility, room-temperature ferromagnetism, and half-metallic behavior. Original data (Table 1) and visualizations (Figures 1, 2) highlight $CdGd_2S_4$'s magnetic superiority and $HgSm_2S_4$'s mechanical advantage. Addressing synthesis and validation challenges will enable their integration into spin valves, sensors, and flexible electronics, advancing next-generation technologies.

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