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Double Hydride Perovskites as Promising Materials for Clean Energy Storage: A First-Principles (DFT) Study

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INTRODUCTION & AIM

Hydrogen is a light, abundant, and clean fuel with great potential for sustainable energy storage and conversion. Among solid-state **hydrogen storage** materials, double hydride perovskites have emerged as promising candidates due to their high hydrogen content, tunable properties, and structural stability. In this study, we investigate **Na_2LiXH_6 (X = Al, Sc, Ga)** double hydride perovskites to explore their **structural, electronic, hydrogen storage, and optical properties**. The goal is to assess their stability and suitability for efficient hydrogen storage applications.

X= Al, Sc, Ga

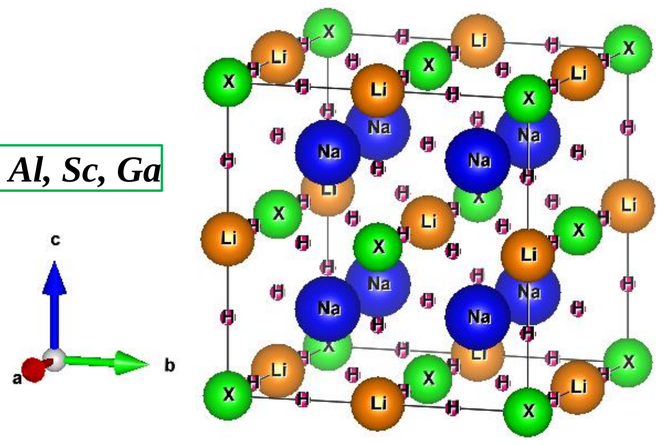

Fig.1. Crystal structure of the **Na_2LiXH_6** (X = Al, Sc, Ga), hydride double perovskites.

Space Groupe : **Fm-3m**

Atoms positions:

H = (0.25, 0, 0)
Li = (0.5, 0.5, 0.5)
X = (0, 0, 0)
Na = (0.25, 0.25, 0.25)

METHOD

- First-principles FP-LAPW method within the DFT framework (***Wien2k package***)
- Exchange-correlation contribution: GGA-PBE approximation

RESULTS & DISCUSSION

1. Structural and Hydrogen Storage Properties:

Formation Energy: $$\Delta E_f(Na_2LiXH_6) = \sum E_{Na_2LiXH_6} - (2E_{Na} + E_{Li} + E_X + 6E_H)$$

Hydrogen Storage Capacity:

$$C_{wt}(\%) = \left(\frac{\alpha\, m_H}{m_{Host} + \alpha\, m_H}\right)$$

Desorption Temperature:

$$T_d = \left(-\frac{\Delta E_f}{\Delta S}\right)$$

DHP	a(Å)	ΔE_f(eV/atom)	$C_{wt}(\%)$	T_d	E_g(eV) "fig.2"
Na_2LiAlH_6	7.29	− 1.52	7.05	373.9	2.60
Na_2LiScH_6	8.01	− 1.45	5.82	356.8	2.17
Na_2LiGaH_6	7.35	− 1.37	4.71	337.1	0.66

Table.1.. a(Å) lattice parameter, ΔE_f formation energy, $C_{wt}(\%)$ hydrogen storage capacity, T_d desorption temperature and E_g(eV) gap energy of Na_2LiAlH_6, , Na_2LiScH_6, and Na_2LiGaH_6

RESULTS & DISCUSSION

3. Electronic properties:

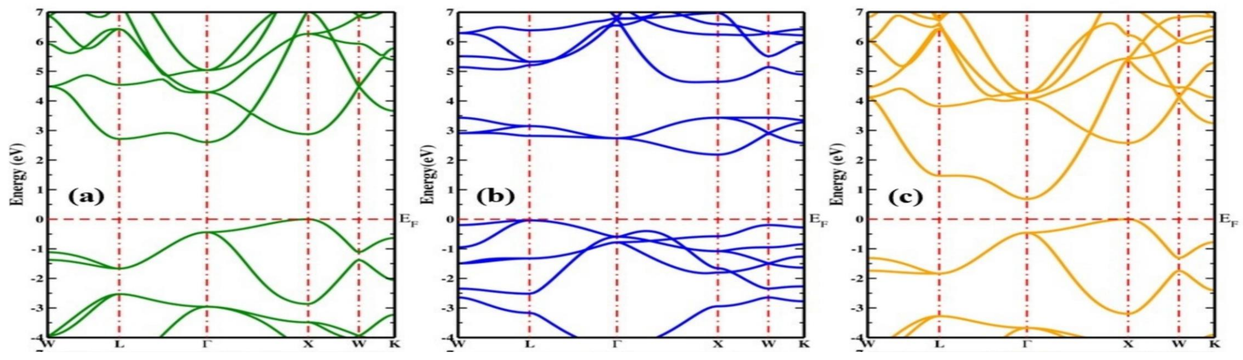

Fig.2.. Band structures obtained using PBE-GGA for (a) Na_2LiAlH_6, (b) Na_2LiScH_6, and (c) Na_2LiGaH_6

3. Optical Properties:

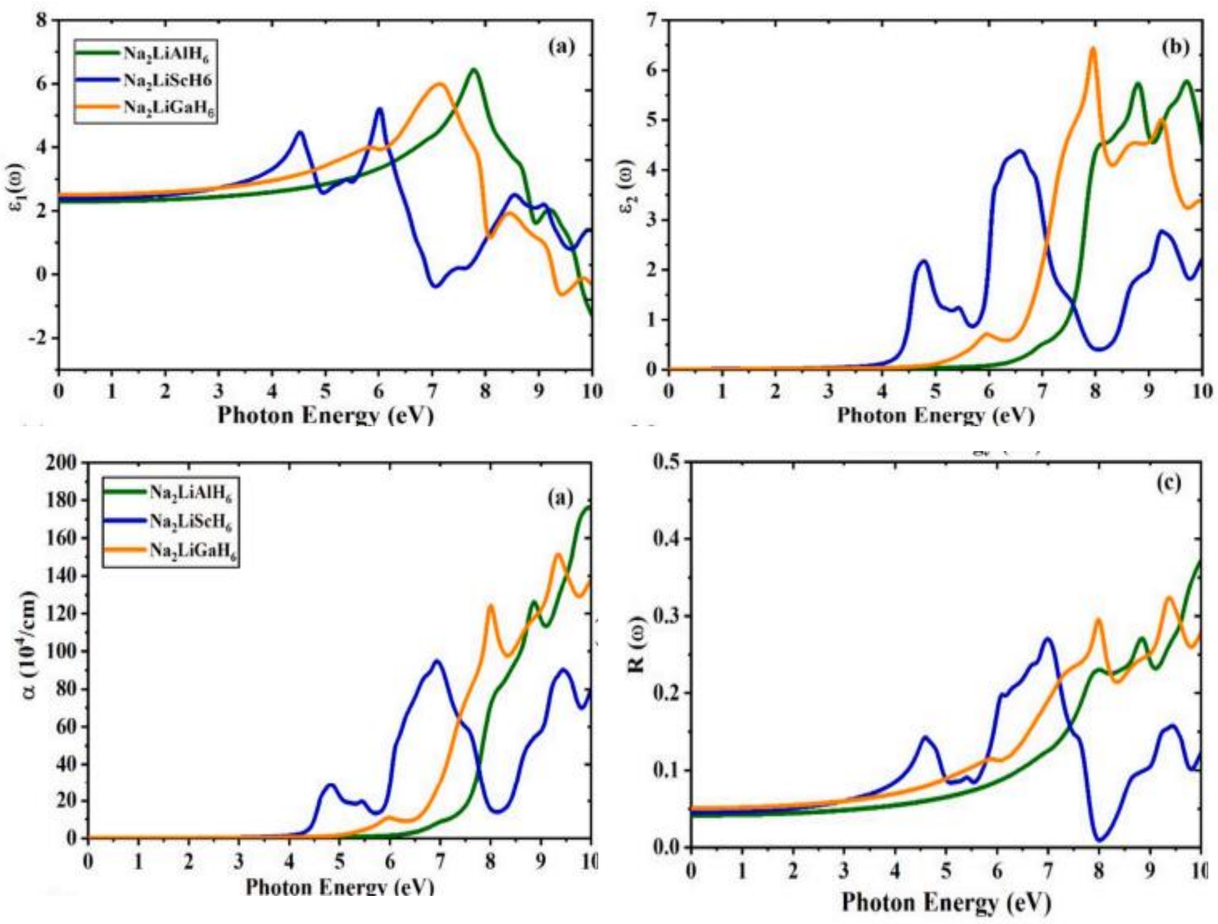

Fig.2.. Optical properties of Na_2LiAlH_6, Na_2LiScH_6, and Na_2LiGaH_6 using PBE-GGA

CONCLUSION

This study investigates the structural, electronic, and optical properties of double hydride perovskites Na_2LiXH_6 (X = Al, Sc, Ga) using first-principles FP-LAPW calculations in Wien2k, revealing dynamically stable cubic structures with indirect band-gap semiconducting behavior suitable for hydrogen storage and optoelectronic applications.

FUTURE WORK / REFERENCES

[1] Ayyaz, Ahmad, et al. "Exploring hydrogen storage potential, thermodynamic, and optoelectronic characteristics of novel double perovskite hydrides Na2LiXH6 (X= Al, Sc, and Ga): DFT analysis." Journal of Energy Storage 122 (2025): 116650.

[2] Ayad, M., et al. "Engineering (Ge/Sn)-Mn halide double perovskites for spintronics, optoelectronics, and energy conversion." Journal of Physics and Chemistry of Solids (2025): 113254.