Study of structural, mechanical, electronic and thermodynamic properties of the N_2CaNa full-Heusler alloy using DFT approach

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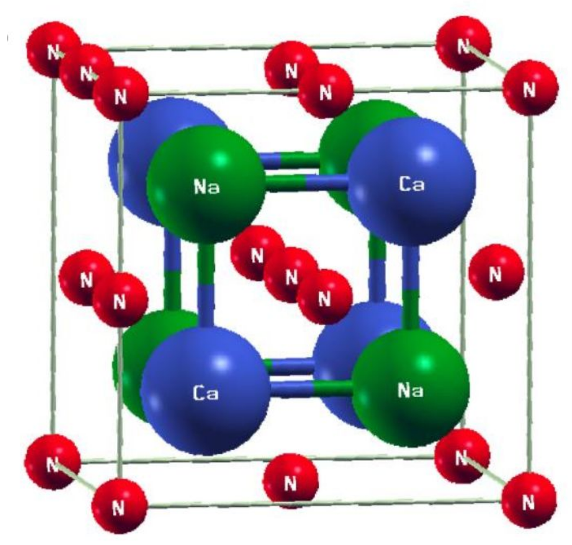
1. Introduction

This study applies density functional theory (DFT) to comprehensively analyze N_2CaNa's (Fig. 1.) properties, establishing its potential for practical applications. DFT calculations allow us to investigate the atomic structure and electronic interactions from first principles, offering accurate predictions of properties such as stability, electronic band structure, and thermodynamic behavior.

Fig. 1. Crystal structure (ball and stick arrangement) of the Half-Heusler C_2CaNa.



2. Methodology

The DFT calculations were conducted using the Vienna Ab initio Simulation Package (VASP), chosen for its efficient plane-wave basis set and projector augmented wave (PAW) method. The Perdew-Burke-Ernzerhof (PBE) generalized gradient approximation (GGA) was used for the exchange-correlation function, and an energy cutoff of 500 eV ensured accurate wavefunction representation. We also used Quantum ESPRESSO for specific thermodynamic calculations. Key input parameters included:

- ***Lattice Structure and K-Point Mesh:*** A face-centered cubic (FCC) Bravais lattice and an 8x8x8 Monkhorst-Pack k-point grid were applied to model the crystal structure accurately.
- ***Convergence Settings:*** Electronic convergence was set to 10-6eV with force convergence at 0.01 eV/Å for each atom.

Structural optimization was achieved through the third-order Birch-Murnaghan equation of state, optimizing lattice constants and minimizing energy. Electronic band structure and DOS were calculated to explore the alloy's electronic characteristics. Mechanical properties were derived from elastic constants, bulk modulus, and shear modulus values, while thermodynamic properties were assessed using Debye and Einstein models to predict stability across temperatures.

3. Results and discussion

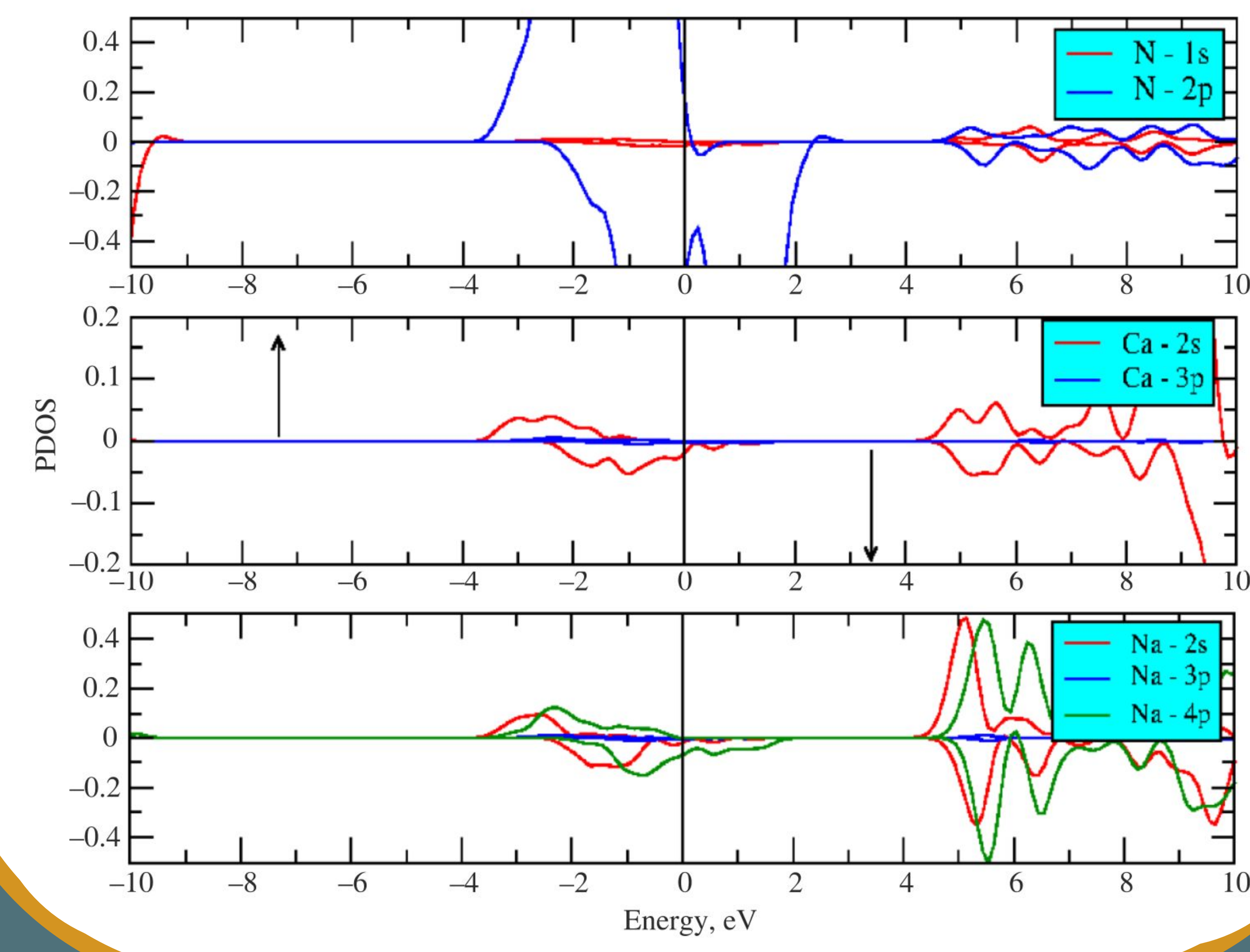
N_2CaNa displayed [Table 1] a stable structure with an equilibrium lattice constant of approximately 5.94 Å. The formation energy, calculated as 29.90 eV, confirmed its energetic favorability and crystallographic stability, both essential for applications requiring resilient materials. The electronic band structure revealed half-metallicity, with metallic behavior in the majority spin channel and a narrow bandgap (~5.08 eV) in the minority channel. This distinct feature allows N_2CaNa to conduct spin-polarized electrons, a valuable property for spintronics where data is processed via electron spin rather than charge.

Compound	a_0, Å	B, GPa	B', GPa	Eg, eV
N_2CaNa	5,94376	61,6	4,95	29,9

Table. 1. Calculated lattice constant (ao), bulk modulus (B), and pressure derivative (B') of half-Heusler alloy N_2CaNa

The DOS further corroborated this, with significant contributions from nitrogen 2p, calcium 2s, and sodium 4p orbitals near the Fermi level (Fig. 2.). Such hybridization between atomic states contributes to N_2CaNa's potential in spin-based electronic applications, enabling efficient data storage and processing. The calculated elastic constants and bulk-to-shear modulus ratio (B/G = 4.77) suggest that N_2CaNa is ductile, compliant with Born's stability criteria, and capable of withstanding stress without fracturing. The bulk modulus of approximately 60.6 GPa and Young's modulus of 35.6 GPa indicate a moderate stiffness and resistance to deformation, making N_2CaNa viable for structural applications where materials must absorb mechanical energy and resist fracture. Thermodynamic stability was examined via heat capacity and entropy calculations across temperature ranges, with results aligning with the Debye T^3 law at low temperatures and the Dulong-Petit law at high temperatures. This behavior suggests that N_2CaNa remains stable under varying thermal conditions, making it suitable for applications requiring thermal resilience, such as electronics where consistent thermal management is critical.

Fig. 2. Electronic density of states (DOS) of the elements N, Ca, and Na. They show their p- and s-orbital, respectively.



4. Conclusion

The DFT analysis of N_2CaNa confirms its potential as a versatile material with wide-ranging applications. Structural stability, half-metallic electronic behavior, mechanical flexibility, and thermodynamic resilience collectively position N_2CaNa as a promising candidate for spintronic, structural, and high-temperature applications. Future experimental studies are recommended to validate these theoretical findings and explore real-world feasibility. Given the alloy's unique properties, N_2CaNa could transform next-generation devices requiring high-performance materials with specialized electronic and mechanical traits.