First-principles Calculations of the Physical Properties and Stability of ScN

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Introduction

Today, the world is widely interested in studying the rare earth nitride materials due to their important physical properties. The hardness of most rare earth nitrides are usually unstable at ambient conditions [1], therefore, we employed the theoretical calculation represented by the first principle technique for discover more properties about the rare earth nitrides. The goal of the present work is using the ab initio calculation to reveal more information and details of the compound ScN stability and properties.

Theoretical Study

These calculations have been performed using the full- potential (linerized) augmented plane wave (lapw+local orbital) [2,3] approach to the density functional theory[4] implemented in WIEN2k code [5], within the Generalized Gradient Approximation through Perdew-Burek-Eneerhof(GGA-PBE), which is used for treatment the electronic exchange-correlation energy function [6].

Results and Discussion

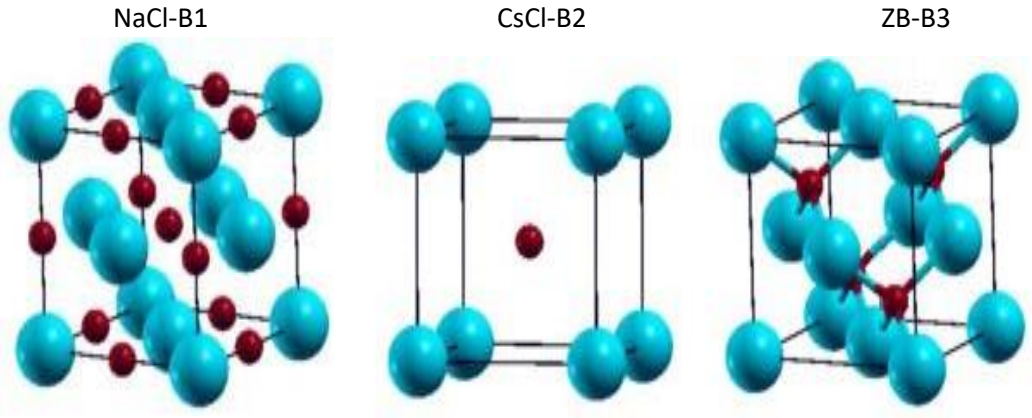

Fig.a: Unit cell of different cubic phases of rare earth nitrides ScN, the blue circles represent the Sc and red one represent the Natom.

Structural properties: The structural stability of the compound of rare earth nitride is analyzed among the three considered NaCl (B1), CsCl (B2), and ZB (B3) (figure b) and it observed that B1 structure is the most stable for the three cubic structures at the ambient conditions.

Electronic properties: It can be seen from the figure c that band gap exists for the two structures B1 and B3, forthe B1 structure there two bandgab direct 2.721eV and 1.2eV at Γ and X respectively, also there is a smaller ndirect Γ-X bandgap with the Fermi level, about the B2 structure we can observed the are two direct band gab 2.68 eV at X and 2.45eV at W, and no bandgap in B2 strucure.

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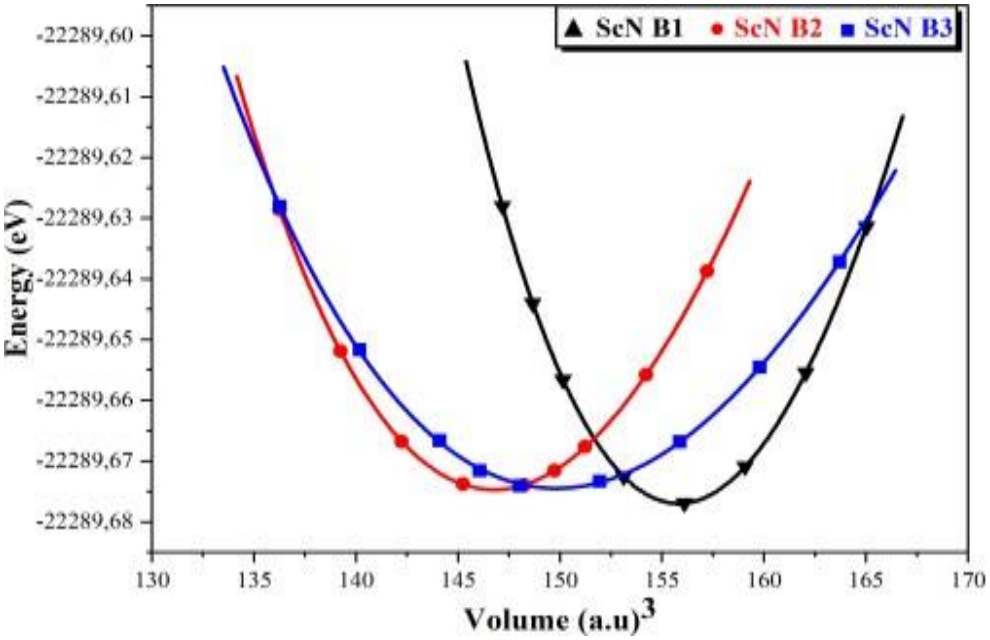

Fig.b Total energy (in eV) versus reduced volume for the three cubic phases of rare earth nitride ScN.

Table 1. Calculated lattice parameter a (Å), total energy E(eV), elastic constants C11, C11, C44 (GPa), bulk modulus B(GPa), Shear modulus B'(Gpa), Young's modulus E (GPa),Poisson's ratio v, for ScN in B1, B2 and B3 structures.

	B1	B2	B3
a (Å)	4.52	2.79	4.91
E_0 (eV)	-22289.61	-22287.51	-22288.98
C11	393.59	523.4258	175.994
C12	104.02	10.69	122.976
C44	165.88	-118.32	95.329
B (GPa)	200.55	181.60	140.615
B' (GPa)E	157.09	-126.66	54.303
(GPa)	373.70	-495.07	151.349
v	0.189	0.954	0.320

B1 B2 B3

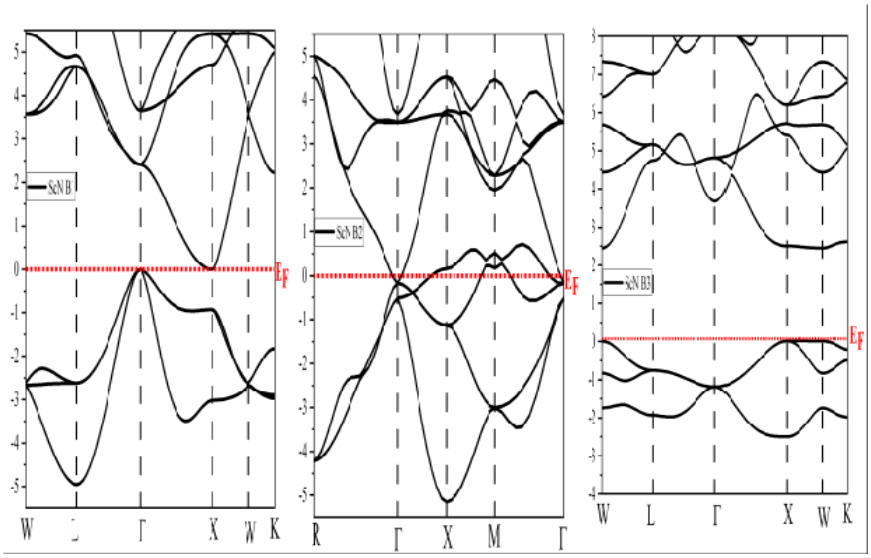

Fig.c: Electronic band structure of ScN in the NaCl(B1), CsCl (B2) and ZB (B3) cubic phases**.**

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Conclusion

In conclusion, the structural, electronic properties of rare earth nitride ScN with three cubic possible structures are analyzed. ScN exhibit a semiconctor nature in B1 and B3 structures, and metallic behavior in B2 structure. The rare earth nitride ScN is found the to be stable structurally and mechanically in NaCl (B1) structure. The calculated results are in good agreement with the available results.

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