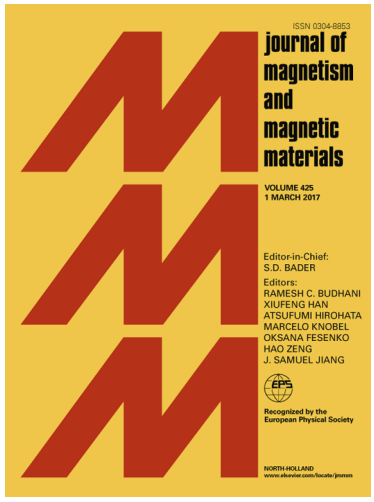


Research articles

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# Magnetic Behavior Study of Samarium Nitride using Density Functional Theory

Narayan N. Som[1], Venu H. Mankad[2], Shweta D. Dabhi[2], Anjali Patel[1] and Prafulla K. Jha[1,*]

[1]*Department of Physics, Faculty of Science, The M. S. University of Baroda, Vadodara 390002, India*
[2]*Department of Physics, Maharaja Krishnakumarsinhji Bhavnagar University, Bhavnagar 364001, India*

**Email: prafullaj@yahoo.com, venumankad@gmail.com**

## ABSTRACT

In this work, the state-of-art density functional theory is employed to study the structural, electronic and magnetic properties of samarium nitride (SmN). We have performed calculation for both ferromagnetic and antiferromagnetic states in rock-salt phase. The calculated results of optimized lattice parameter and magnetic moment agree well with the available experimental and theoretical values. From energy band diagram and electronic density of states, we observe a half-metallic behaviour in FM phase of rock salt SmN in while metallicity in AFM I and AFM III phases. We present and discuss our current understanding of the possible half-metallicity together with the magnetic ordering in SmN. The calculated phonon dispersion curves shows dynamical stability of the considered structures. The phonon density of states and Eliashberg functional have also been analysed to understand the superconductivity in SmN.

**Keywords:** Density functional theory, Samarium nitride, electronic band structure, magnetic, phonons, superconductivity.