

Magnetic moment and Magnetocrystalline anisotropy of Fe_{16}N_2 : A first principles study

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Using the full potential linearized augmented plane wave (FLAPW) method, we have investigated the electronic structure and magnetic properties of Fe_{16}N_2 with body centered tetragonal structure. The average magnetic moment was found to be $2.5 \mu_{\text{B}}/\text{Fe}$ atom which is in agreement with the experimentally calculated value. A perpendicular magnetocrystalline anisotropy of 0.57 MJ/m^3 was obtained for pure Fe_{16}N_2 which is due to the tetragonal distortion and it is in agreement with earlier reported results. The estimated coercivity and maximum energy product are 6.5 kOe and 71.7 MGOe.