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 $\mu_B$/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.