

Electronic structure and magnetic properties of $\text{Nd}_2\text{Fe}_{14}\text{B}$: A first principles study

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We have studied the electronic structure and magnetic properties of $\text{Nd}_2\text{Fe}_{14}\text{B}$ by using the full potential linearized augmented plane wave method implemented in Wien2k code. A DFT+U scheme was applied to treat the localized 4f electrons of Nd. It is observed that the antiferromagnet (AFM) configuration between Fe and Nd sublattice is more stable than the ferromagnetic (FM) and the difference between AFM and FM was 940 meV. The total magnetic moment was found to be $36.48 \mu_B/\text{f.u.}$, which is in good agreement with the experimentally reported value.

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