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Electronic, Magnetic and Mechanical Properties Of Nd2Fe14B Permanent Magnets: Ab Initio Study

Neodymium-based permanent magnets (Nd2Fe14B) are the potential permanent magnets for use in various applications due to their high magnetic field strength and resistance to demagnetisation. These magnets have various applications in highly efficient energy conversion machines and devices such as wind turbines and electric vehicles due to their exceptional magnetic properties. However, they suffer from low operating temperatures below 585 K. In this study, we investigate the electronic, magnetic and mechanical properties of Neodymium magnets using the first principle density functional theory approach. Nd2Fe14B was found to be thermodynamically stable since the heats of formation are found to be negative. However, it was found that Nd2Fe14B fails to meet the tetragonal stability criteria, which is ascribed to the mechanical instability of the material. Moreover, the density of states was calculated to predict the electronic stability of the permanent magnets which is in agreement with the calculated heats of formation. The phonon dispersion curves were also calculated and Nd2Fe14B is found to be vibrationally unstable due to the presence of soft modes. The calculated magnetic moment compares well to the experimental findings. The substitution of Nd with available rare earth elements is suggested to enhance the stability and magnetic properties of the magnets.

Apply to be considered for a student ; award (Yes / No)?

Yes

Level for award;(Hons, MSc, PhD, N/A)?

PhD

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