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First principle study on the magnetic properties and electronic structure of Ce and Dy substituted on Nd2Fe14B permanent magnet.

The development of new rare-earth free Nd-Fe-B permanent magnet remains a serious issue for the transition to a green and sustainable world, as permanent magnets are an important component in the design and development of highly-efficient energy conversion machinery and devices. The effects of Ce and Dy on the electronic structures and magnetic properties of Nd2Fe14B have been studied using the density function theory (DFT) within the generalized gradient approximation (GGA). Results are presented for the total density of states (DOS), orbital-decomposed, and spin-decomposed partial DOS. The study showed that Ce slightly decreased the magnetic properties of Nd2Fe14B magnet. On the other hand, Dy decreases the magnetic moments of the magnet. The study revealed that both Cerium and Dysprosium affects the properties of permanent magnets. The calculated spin-magnetic moments on each of the six Fe sites are in good agreement with the values deduced from the neutron scattering experiment.

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

Yes

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

MSc

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