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Effects of Earth Metal Dopants on the Properties of a Neodymium Magnet Using a First-Principles Approach.

Rare-earth (RE) ions enhance the stability of permanent magnets against demagnetization, making them vital in wind turbines, electric vehicle engines, magnetic resonance imaging machines, and cell phone devices. However, the rising costs and dwindling reserves of RE materials necessitate the development of RE-free permanent magnets for a sustainable economy. This study uses first-principles calculations to investigate the magnetic properties and electronic structure of $RE_2Fe_{14}B$ (RE = Nd, Dy, Y, La, and Ce). Spin-polarized density functional theory, using the generalized gradient approximation and Perdew–Burke–Ernzerhof
function was performed to predict the properties of $RE_2Fe_{14}B$ permanent magnets. The study found that the spin and orbital magnetic moments of Nd, Dy, Y, La, and Ce atoms are opposite, consistent with Hund's rule, with the total orbital magnetic moment exceeding the total spin magnetic moment. Y prefers the 4f site, while La prefers the 4g site. Ce showed specific magnetic moments at the 4f and 4g sites, contributing oppositely to the total magnetic moment. Substitutions of nonmagnetic La and Ce
reduced the total magnetic moments of the cells. The bandwidth of the Fe d states in $La_2Fe_{14}B$ is shorter than those of the Nd, Dy, Y, and Ce structures because the lattice parameter of $La_2Fe_{14}B$ was more significant than those of all other structures. The findings align well with previous experimental and theoretical data, indicating that substituting Dy, Y, La, and Ce affects the properties of permanent magnets, where Ce has the highest magnetic moments and Dy has the highest Curie temperature compared to the other RE substitutes.

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