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## The effect of Ce and Gd on the magnetic and mechanical properties of Nd<sub>2</sub>Fe<sub>14</sub>B permanent magnets

Neodymium-based permanent magnets (Nd<sub>2</sub>Fe<sub>14</sub>B) can be used in various applications, such as electric vehicles and wind power generators, due to their high magnetic field strength and demagnetisation resistance. However, they suffer from low operating temperatures below 585 K and poor mechanical properties. This study investigates the effect of rare earth elements such as Gd and Ce on the Nd<sub>2</sub>Fe<sub>14</sub>B magnets. Their structural, electronic, mechanical and magnetic properties were calculated using the ab initio density functional theory approach. Heats of formation were used to mimic the thermodynamic stability of the magnets and predicted that NdCeFe<sub>14</sub>B was the most stable. The partial substitution of Nd with Gd improves the ductility, mechanical stability, magnetic strength and operation temperature of Nd<sub>2</sub>Fe<sub>14</sub>B permanent magnets. These findings provide insight into the future development of permanent magnetic compounds with good mechanical properties and high operation temperatures.

### Apply for student award at which level:

None

### Consent on use of personal information: Abstract Submission

Yes, I ACCEPT

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