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First Principles Calculation of Formation Energy for Nd-Fe-B compounds ADIE HANINDRIYO, Japan Adv Inst of Sci and Tech, SOUMYA SRIDAR, K.C. HARI KUMAR, Indian Institute of Technology Madras, RYO MAEZONO, Japan Adv Inst of Sci and Tech — The compound $Nd_2Fe_{14}B$ is widely used in manufacturing permanent magnets. This interest has driven much of the research on the Nd-Fe-B system including the computational calculation of phase diagrams (CALPHAD). Formation energy of Nd-Fe-B compounds is required for CALPHAD input, and are calculated using Density Functional Theory (DFT). Hubbard U correction is used to account for the localized nature of Nd 4f electrons. Comparison between 2 methods of choosing Hubbard U value is drawn: a simplified implementation of DFT+U using effective Hubbard U value (U_{eff} = U-J) and from constrained random phase approximation (cRPA) for bulk Nd. It is shown that the former method is insufficient to accurately calculate formation energy of several Nd-Fe-B compounds. Comparison is also drawn between 2 types of pseudopotentials, norm-conserving and ultrasoft pseudopotentials.

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