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Site-preference and valency for rare-earth sites in (R-Ce)2Fe14B [R=La,Nd] magnets[1] AFTAB ALAM, Ames Laboratory, Ames Iowa, MAHMUD KHAN, Ames Laboratry, Ames Iowa, R.W. MCCALLUM, D.D. JOHNSON, Ames Laboratory and Iowa State University, Ames Iowa — Rare-earth (R) permanent magnets of R2Fe14B have technological importance due to their high energy products, and they have two symmetry distinct R-sites (Wyckoff 4f and 4g) that affect chemistry and valence. Designing magnetic behavior and stability via alloying is technologically relevant to reduce critical (expensive) R-content while retaining key properties; cerium, an abundant (cheap) R-element, offers this potential. We calculate magnetic properties and Ce site preference in (R1-xCe_x)Fe14B [R=La,Nd] using density functional theory (DFT) methods. The Fe moments compare well with neutron scattering data – remain weakly affected by Hubbard U, but improved with spin-orbit coupling. In (La,Ce)2Fe14B, Ce alloys for $0 < x < 1$ with a preference for smaller R(4f) sites, as observed, a trend we find unaffected by valence. Whereas in (Nd,Ce)2Fe14B, Ce is predicted to have limited alloying ($x < 0.3$) with a preference for larger R(4g) sites, resulting in weak partial ordering and segregation. Curie temperatures versus x were predicted for a typical sample processing and verified experimentally. We shall also present some initial results on the critical mixed valency of Ce in related compounds.

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