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Qualitative aspects of magnetism formation in Gd and its compounds KIRILL BELASHCHENKO, University of Nebraska-Lincoln, VLADIMIR ANTROPOV, GERMAN SAMOLYUK, Ames Laboratory — Using highly precise full-potential electronic structure calculations, we study the formation of magnetism in gadolinium. By manipulating the 4f-shell magnetic moments in a large supercell, the interplay between on-site and off-site contributions to the spin polarization of valence electrons is analyzed. Qualitative features of exchange coupling are discussed, and the limitations of model RKKY-like approaches are demonstrated. We also analyze the magnetization density distribution in ferromagnetic hcp Gd which, unlike transition-metal ferromagnets, shows a strongly inhomogeneous, directional structure in the interstitial region. The qualitative features revealed in this study are very generic, and we discuss their relevance to other rare-earth elements and their compounds.

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