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Structure and Magnetic Properties of Rare Earth Doped Transparent Alumina KRISTA LIMMER, MAHESH NEUPANE, TANYA CHANTAWANSRI, US Army Rsch Lab - Aberdeen — Recent experimental studies of rare earth (RE) doped alumina suggest that the RE induced novel phase-dependent structural and magnetic properties [1]. Motivated by these efforts, the effects of RE doping of alpha and theta alumina on the local structure, magnetic properties, and phase stability have been examined in this first principles study. Although a direct correlation between the magnetic field dependent materials properties observed experimentally and calculated from first principles is not feasible because of the applied field and the scale, the internal magnetic properties and other properties of the doped materials are evaluated. The RE dopants are shown to increase the substitutional site volume as well as increasingly distort the site structure as a function of ionic radii. Doping both the alpha (stable) and theta (metastable) phases enhanced the relative stability of the theta phase. The energetic doping cost and internal magnetic moment were shown to be a function of the electronic configuration of the RE-dopant, with magnetic moment directly proportional to the number of unpaired electrons and doping cost being inversely related.
[1] Pavlacka, Robert, et al. Ceramic Transactions 252: 3, 2015.

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