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Temperature-composition phase diagrams of Gd-doped EuO and EuS JOONHEE AN, Dep. of Physics and Astonomy, Univ. of Nebraska-Lincoln, S. BARABASH, Dep. of Materials Science and Engineering, Univ. of California, Los Angeles, K. BELASHCHENKO, Dep. of Physics and Astonomy, Univ. of Nebraska-Lincoln — We have computed the temperature-phase diagram of $Eu_{1-x}Gd_xO$ alloys by combining density functional theory in the generalized-gradient approximation with Hubbard U correction on f-orbitals with the regular cluster expansion and Monte-Carlo approach. The cluster expansion fit has been performed with varying numbers of distinct cluster types until the formal cross-validation score is minimized. Our results indicate that (i) pair interactions are relatively stronger than other cluster types, (ii) the pair terms decay rapidly with distance up to 10 Å, (iii) the pair terms are attractive for direct interactions between cations and repulsive for indirect interactions through anions, and (iv) the calculated convex hull is asymmetric about x=0.5, displaying more deep ground states in Eu-rich regions than in Gd-rich regions. The asymmetry of the convex hull may imply relative instability of Gd-rich compounds, as was shown by previously-reported experimental difficulties to make Gd-rich compounds. A comparison with a similar binary system - sulfur replacing oxygen - is made, showing that both oxides and sulphides are dominated by deformation interaction. The sulphides have a marginal tendency to phase-separate into pure compounds at low temperatures, whereas the oxides tend to order.

Joonhee An
Dep. of Physics and Astonomy, Univ. of Nebraska-Lincoln

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