

Abstract Submitted
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Unusual magnetism of Gd_5Ge_4 with non magnetic rare earths substitutions¹ DURGA PAUDYAL, The Ames Laboratory, US Department of Energy, Iowa State University, Ames, IA 50011-3020, USA, Y. MUDRYK, V.K. PECHARSKY, K.A. GSCHNEIDNER, JR., The Ames Laboratory, U. S. Department of Energy, Iowa State University, Ames, IA 50011-3020, USA — We present first principles and experimental studies on the small substitutions of Gd atoms by Lu, La, Y, and Sc atoms in Gd_5Ge_4 . While replacing the Gd atoms located inside the slabs with the Lu or Y atoms leads to a substantial loss of ferromagnetism, the identical substitutions of other Gd locations preferred by La atoms have essentially no effect on the magnetostructural transitions. On the other hand, the Sc atoms prefer the same locations as the Lu and Y atoms. This substitution, however, changes the crystal structure of Gd_5Ge_4 from Sm_5Ge_4 type to Pu_5Rh_4 type at 25% of Sc which was not observed with the former substitutions. The Pu_5Rh_4 -type has structural parameters that are intermediate between the Gd_5Si_4 and Sm_5Ge_4 types. The exchange interactions in this substitution are positive which indicates that the Sc substituted Gd_5Ge_4 has the ferromagnetic ground state.

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