Origins of ferromagnetism and antiferromagnetism in Gd$_5$Ge$_4$\textsuperscript{1}  
DURGA PAUDYAL, V.K. PECHARSKY, K.A. GSCHNEIDNER, JR., The Ames Laboratory, U. S. Department of Energy, Iowa State University, Ames, IA 50011  — The origin of ferromagnetism appearing as a result of a magnetic-field-induced first-order phase transition in Gd$_5$Ge$_4$ is explored by calculating the total energy, local exchange splitting, density of states, and magnetic moments. The calculations were performed using density functional approaches including the on-site Coulomb interaction parameter. The total energy as a function of shear distortion along the $a$ axis for two different orthorhombic structures is in agreement with experiment, indicating a first-order magnetostructural transition in Gd$_5$Ge$_4$. The rearrangement of Gd 5$d$ and Ge 4$p$ densities of states, the substantial differences in atom-projected band energies, the exchange splitting, and the magnetic moments calculated with ferromagnetic spin arrangements in the orthorhombic Sm$_5$Ge$_4$-type and Gd$_5$Si$_4$-type structures of Gd$_5$Ge$_4$ help to clarify the differences in the magnetic states of these two structures. Our calculations indicate that the Sm$_5$Ge$_4$-type structure of Gd$_5$Ge$_4$ is the structural ground state and that it is antiferromagnetic.

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