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Origins of ferromagnetism and antiferromagnetism in Gd_5Ge_4[1]
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— The origin of ferromagnetism appearing as a result of a magnetic-field-induced first-order phase transition in Gd_5Ge_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_5Ge_4. The rearrangement of Gd 5d and Ge 4p 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_5Ge_4-type and Gd_5Si_4-type structures of Gd_5Ge_4 help to clarify the differences in the magnetic states of these two structures. Our calculations indicate that the Sm_5Ge_4-type structure of Gd_5Ge_4 is the structural ground state and that it is antiferromagnetic.

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