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Non-collinear magnetism of GdB_4: A DFT+U study[1] M. N. HUDA, LEONARD KLEINMAN, Department of Physics, University of Texas at Austin, Texas-78712, USA — Lanthanide-borides show antiferromagnetic behavior where the magnetocrystalline anisotropy plays a major role in their magnetic structures. A recent neutron scattering experiment showed a particular noncollinear behavior of GdB_4 at room temperature. We will present our study on the non-collinear magnetism of GdB_4 with the GGA + U method with spin orbit coupling. We have found that with or without spin-orbit coupling and with Ucollinear magnetism is favorable by few meV than the experimentally found noncollinear magnetic configuration. Among the noncollinear magnetism configurations that we have studied, when a Uparameter and spin-orbit coupling are considered, the experimentally found noncollinear configuration was found to be favorable. However, the value of U parameter is not unique; a range of values were able to get this magnetic order.

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