

Abstract Submitted
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GGA+ U calculation of the magnetic ground state of GdB₄¹
LEONARD KLEINMAN, MUHAMMAD HUDA², University of Texas — We have studied eight collinear and non-collinear magnetic orientations of GdB₄ using the GGA + U method, without and with spin-orbit coupling, for values of $U - J$ between 0 and 6. For $U - J = 6$, the value which had been found to yield the correct Gd lattice constants, we obtain GdB₄ lattice constants within 0.26% of experiment. We find the magnetization lies in-plane but is collinear, in disagreement with the most recent experimental determination.

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²Current address: National Renewable Energy Laboratory

Leonard Kleinman
University of Texas

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