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Theoretical study of electronic and magnetic properties of GdRhIn with strong electron correlations

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INTRODUCTION & AIM

RTX compounds [1,2] are versatile materials showing promising magnetic properties, including the magnetocaloric effect (MCE) for refrigeration applications. The compound GdRhIn is a notable example, recently shown to undergo an antiferromagnetic-to-ferromagnetic transition at 16 K before becoming paramagnetic at 34 K. This behavior yields a large MCE, with a significant magnetic entropy change. However, the electronic structure of GdRhIn remains unexplored. In this work, we report theoretical calculations of the electronic and magnetic properties of GdRhIn to provide a deeper understanding of its fundamental behavior [3].

METHODS AND CRYSTAL STRUCTURE

COMPUTATION

- **Method:** DFT+U
- **Software package:** Quantum ESPRESSO
- **Functional:** GGA-PBE
- **Coulomb parameter U for Gd:** 6.7 eV
- **Exchange parameter J for Gd:** 0.7 eV
- **Cutoff:** 60 Ry
- **k-mesh:** 12×12×12

CRYSTAL STRUCTURE

- **Prototype:** Fe_2P (Hexagonal)
- **Space Group:** *P*-62m (No. 189)
- **Initial Params:** a = 7.53 Å, c = 3.92 Å

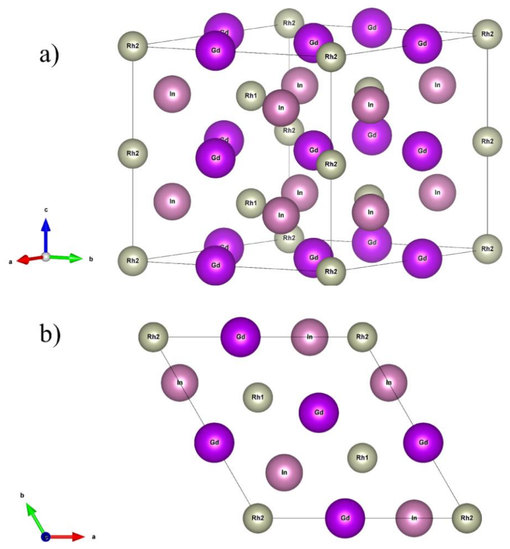

Fig. 1. Crystal structure of GdRhIn: (a) perspective view and (b) view along the *c*-axis. Color coding: Gd (purple), Rh1/Rh2 (silver), In (pink).

RESULTS & DISCUSSION

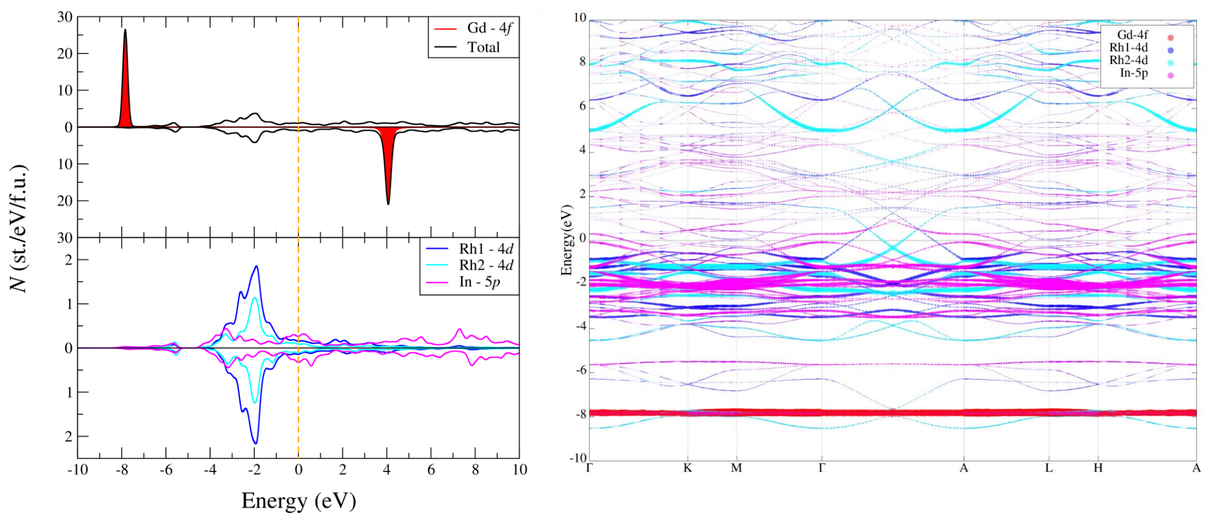

Fig. 2. The total and partial densities of states (left) and the band structure (right) are shown for the majority spin projection in the GdRhIn ferromagnetic state.

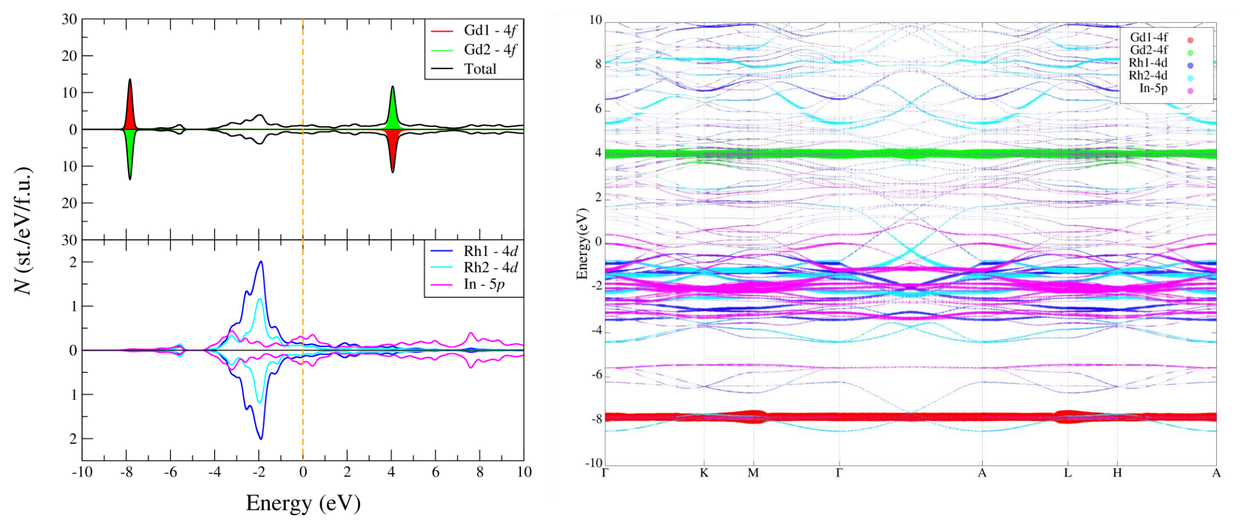

Fig. 3. The total and partial densities of states (left) and the band structure (right) are shown for the majority spin projection in the GdRhIn antiferromagnetic state.

The compound exhibits a ferromagnetic (FM) ground state, though the antiferromagnetic G-type (AFM-G) configuration lies only 3.51 meV/f.u. higher in energy, indicating competing exchange interactions mediated by the RKKY mechanism. This proximity suggests potential magnetic switching under external stimuli, making GdRhIn promising for spintronics and magnetocaloric applications. The A-type and C-type AFM orderings are less stable, lying 2.97 meV/f.u. and 0.76 meV/f.u. above the AFM-G state, respectively. Analysis of the electronic structure reveals strongly localized 4f states of Gd, responsible for the magnetic moment of 7.1 μ_B, in agreement with experimental data. The Rh and In sublattices remain non-magnetic, with the conduction band near the Fermi level formed by hybridized Rh 4d and In 5p states.

The density of states and band structure confirm minimal spin polarization for Rh and In, while the Gd 4f states dominate the magnetic behavior. The FM and AFM-G configurations exhibit nearly identical band dispersions, with only minor differences in the Gd 4f splitting, further highlighting the system's magnetic flexibility. These findings align with experimental observations. The material's tunable magnetic state makes it promising for spintronic and magnetocaloric applications.

CONCLUSION

The electronic and magnetic properties of GdRhIn have been elucidated through DFT+U calculations. The system exhibits a ferromagnetic ground state, but its near-degeneracy with the G-type antiferromagnetic state points to strong competition in exchange interactions, consistent with an RKKY mechanism. This magnetic frustration underpins the material's complex phase transitions and large magnetocaloric effect. The magnetic moment is confirmed to be entirely localized on the Gd sites (7.1 μ_B), with no contribution from Rh or In, providing a solid theoretical foundation for interpreting experimental data.

REFERENCES AND ACKNOWLEDGEMENTS

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