Antiferromagnetism in Cd_6Tb 1/1 periodic approximant crystal from DFT calculations

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We present a comprehensive ab initio study of the electronic structure and magnetic ordering in Cd_6Tb, a 1/1 periodic approximant of a Tsai-type quasicrystal, using density functional theory. This compound is of particular interest as it was the first quasicrystal-related system in which long-range antiferromagnetic order was experimentally observed [1]. Fully relativistic calculations, including spin–orbit coupling and structural relaxation, are employed to identify the magnetic ground state and assess the stability of competing magnetic configurations.

Our results correctly predict an antiferromagnetic ground state. The calculated magnetic moment of 9.3 μ_B per Tb atom is in good agreement with the experimental value of 9.8 μ_B, without the need for DFT+U corrections. We find that Tb magnetic moments preferentially align along a cubic axis, while alternative noncollinear configurations, such as radial and orthoradial associated with the icosahedral geometry are energetically unfavorable by several Ry per atom and computationally unstable.

Structural relaxation mainly affects Cd atoms within the central tetrahedra of Tsai clusters, while Tb positions and magnetic moments remain largely unchanged. Despite the strong localization of Tb 4f states near the Fermi level, their behavior is well captured within standard methods. These findings provide microscopic insight into the origin of antiferromagnetism in Cd_6Tb and establish a reliable first-principles framework for studying magnetism in complex quasicrystalline and approximant systems.

References:

[1] R. Tamura, Y. Muro, T. Hiroto, K. Nishimoto, and T. Takabatake, Phys. Rev. B 82 (2010) 220201