

# Prediction of Magnetic Order and dimensionality in Cerium-Based Compounds Guided by Structural characteristics and tri-critical exponents.

Josh Torres, Jeffery Moore, Jayce Littleton, Anjali Poulo and Tej Nath Lamichhane

Department of Engineering Physics, University of Central Oklahoma

Ce is the most abundant element and exhibits the most diverse chemical and physical properties among the lanthanides. It has immense potential to solve the looming raw materials crisis in high performance magnets industry providing new compounds for gap magnets[1, 2]. The prediction of magnetic order and dimensionality in cerium-based compounds represents a crucial area of research due to its unique magnetic and electronic properties. Here we use structural characteristics and tri-critical exponents to identify the key parameters influencing their magnetic order. By integrating these structural insights with tri-critical exponents derived from experimental and theoretical studies, we develop a predictive model that can accurately determine the magnetic dimensionality and ordering phenomena. Our findings highlight the pivotal role of lattice symmetry, valency, bond lengths, and coordination environments in shaping the magnetic properties. The proposed model not only elucidates the fundamental mechanisms driving magnetic order in cerium-based compounds but also provides a robust comparison framework for designing and comparing new lanthanides[3] and actinides[4] materials with tailored magnetic properties. This approach paves the way for advancements in materials science, particularly in the development of novel magnetic materials alloy for technological applications.

1. Lamichhane, T.N., et al., Single-Crystal Permanent Magnets: Extraordinary Magnetic Behavior in the  $\text{Ta}$ -,  $\text{Cu}$ -, and  $\text{Fe}$ -Substituted  $\text{CeCo}_5$  Systems. *Physical Review Applied*, 2019. 11(1): p. 014052.
2. Lamichhane, T.N., et al.,  $\text{Ce}_3\text{Mg}_x\text{Co}_9$ : Transformation of a Pauli Paramagnet into a Strong Permanent Magnet. *Physical Review Applied*, 2018. 9(2): p. 024023.
3. Churna Bhandari, G.N.N., Jonathan D.H. Smith, Durga Paudyal, Accurate Machine Learning Predictions of Coercivity in High-Performance Permanent Magnets. 2023.
4. Broyles, C.C., William; Sheng Ran, Structure-Driven Prediction of Magnetic Order in Uranium Compounds. 2024.