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Magnetic Structures Database from Symmetry-aided High-Throughput Calculations

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Magnetic structures determine many key properties of magnetic materials, yet they are experimentally known for very limited compounds. Conventional theoretical predictions rely on first-principles total-energy calculations, but these require initial magnetic configurations as input, whose possibilities are in principle infinite, rendering a systematic search impractical. Although Landau theory and symmetry analysis are widely used to classify magnetic ordering through magnetic space groups and irreducible representations (irreps), applying them directly to generate a finite set of candidate magnetic configurations remains a major challenge due to unavoidable residual degrees of freedom. Here we overcome this obstacle by developing an irrep-basis-vector strategy augmented by two physically motivated scenarios: an irrep-compatible maximal-magnetic-subgroup criterion and a high-symmetry moment-direction approximation. Benchmarking our theory against 1,044 Landau-compatible experimentally magnetic structures in MAGNDATA, we find that for the four high-symmetry crystal systems (tetragonal, trigonal, hexagonal, and cubic), only 48 candidates per material on average are sufficient to achieve over 90% coverage, while the overall coverage across all crystal systems reaches 75%. Subsequent DFT calculations achieve an accuracy of 86% on the benchmark subset. Applying this framework to 19,808 stoichiometric transition-metal compounds with fewer than 60 atoms per primitive cell, we construct a magnetic-structure database containing more than 4,000 magnetic materials. Applications to magnetic topology and altermagnetism illustrate the potential utility of this database for future study.