

High-throughput calculations of multiferroic collinear antiferromagnets exhibiting odd-parity responses

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Altermagnets have attracted considerable attention in antiferromagnetic spintronics because they exhibit spin splitting even in the absence of spin–orbit coupling [1, 2], giving rise to responses such as the anomalous Hall effect [3] and spin-current generation [4, 5]. In contrast, antiferromagnets without nonrelativistic spin splitting are classified as conventional antiferromagnets and have received much less attention.

Against this background, we have shown that even among conventional antiferromagnets, there exist multiferroic collinear antiferromagnets in which polarity or chirality is induced by magnetic order, leading to odd-parity responses driven by conventional antiferromagnetism [6]. However, a search of MAGNDATA based on the symmetry conditions satisfied by such multiferroic collinear antiferromagnets revealed that most candidate materials have low transition temperatures or complicated crystal structures, making them unsuitable as model materials.

In this study, we performed high-throughput calculations using a magnetic structure generation method based on spin space groups, which we have recently developed [7]. Specifically, we investigated the most stable magnetic structures of ICSD materials containing 3d transition-metal elements, namely Cr, Mn, Fe, Co, and Ni.

As a result, we identified several materials that can exhibit odd-parity responses induced by conventional antiferromagnetism. In addition, we constructed tight-binding effective models for these candidate materials and evaluated their odd-parity responses.

These results demonstrate the usefulness of spin space group-based magnetic structure generation for materials exploration in antiferromagnetic spintronics and provide a new guiding principle for the discovery of antiferromagnetic spintronic materials.

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