"Solving symmetry constraints and diagnosing band topology for all 1,651 magnetic space groups"

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Abstract: Symmetries have played a central role ever since the inception of band theory in the 1930s. The full tabulation of all symmetry transformation rules possible in a crystal was achieved in the 1960s-70s, and one might consider this problem completely solved. The recent advent of band topology, however, rekindled interest in this problem. Armed with new insights from topological band theory, we revisit the 80-year-old problem of band symmetry. In this talk, I will argue that a fundamental aspect of band symmetry, concerned with its global properties over the Brillouin zone, has been largely overlooked. First, I will describe how the set of symmetry-respecting band structures should be viewed as a mathematical lattice (an abelian group). Next, I will argue that by contrasting the full set of band structures against those having a simple real-space description, one can efficiently isolate topologically nontrivial band insulators and semimetals, for all 1,651 magnetic space groups.