

Algebraic search for cooperative-rotational rigid-unit modes

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Crystalline solids consisting of three-dimensional networks of interconnected rigid units are ubiquitous amongst functional materials. And in many cases, application-critical properties are sensitive to rigid-unit rotations at low-temperature, high pressure, or strategic stoichiometry. However, the shared atoms that connect rigid units impose severe constraints on any rotational degrees of freedom, which must then be cooperative throughout the entire network. Successful efforts to identify cooperative-rotational rigid-unit modes (RUMs) in crystals have employed split-atom harmonic potentials, exhaustive testing of the rotational symmetry modes allowed by group representation theory, and even simple geometric considerations. Here, we present a purely algebraic approach to RUM identification wherein the conditions of connectedness are used to construct a linear system of equations in the rotational symmetry mode amplitudes.

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