

Abstract Submitted
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Algebraically Determining Rigid Unit Modes¹ SHAE MACHLUS,
Florida State University — Application-critical properties of crystals are often either inhibited or permitted by rigid unit modes (RUM's). RUM's are tilting patterns in crystal lattices that displace atoms, and they signify structural phase transitions between polymorphs of a given crystal. Previous efforts have been made to identify RUM's in several important materials classes. Strategies have been employed such as ball-and-spring simulations, phonon-frequency calculations, and trial-and-error searches. But no methodology has been as simple or exhaustive as the algebraic approach developed by Prof. Branton Campbell's group at Brigham Young University during the past year.

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