Systematic Discovery of Noncentrosymmetric Materials

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Abstract: Symmetry is a fundamental concept uniting science and art, resulting in a natural abundance of centrosymmetric (CS) structures in crystalline solids. Nevertheless, noncentrosymmetric (NCS) materials are highly sought after due to their remarkable structure-property correlations. Specifically, properties like piezoelectricity, pyroelectricity, second-harmonic generation, and ferroelectricity make them indispensable for applications ranging from medical lasers and telecommunications to lithography, energy harvesting, detectors, and data storage. The challenge lies in achieving the large-scale synthesis of NCS structures, despite efforts to utilize NCS chromophores such as distorted polyhedra, polarizable metals, or asymmetric anions. The thermodynamic preference for symmetry often leads to CS products. This presentation will examine the key factors that dictate the formation of framework structures and macroscopic centricity by analyzing the structural nuances of novel compounds containing asymmetric building blocks. We will also discuss strategic approaches to streamline the development of functional solid-state materials with NCS characteristics.

References

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