

# Systematic Discovery of Noncentrosymmetric Materials

Kang Min Ok

*Department of Chemistry, Sogang University*

Email: kmok@sogang.ac.kr

## Abstract

In both science and art, symmetry is a fundamental concept. This explains why centrosymmetric (CS) structures are so common in crystalline solids. However, noncentrosymmetric (NCS) materials are highly desirable because of their strong link between structure and function.

These materials are crucial for applications in medical lasers, telecommunications, lithography, energy harvesting, detectors, and data storage, attributable to properties such as piezoelectricity, pyroelectricity, second-harmonic generation, and ferroelectricity.

Despite the use of NCS building blocks—such as distorted polyhedra, polarizable metals, or asymmetric anions—synthesizing these NCS structures on a large scale remains a challenge. The reason is that thermodynamics often favors the creation of more symmetric, CS products. This presentation will delve into the critical factors that govern how framework structures form and what determines their overall symmetry. We will do this by examining the intricate structures of new compounds made with asymmetric building blocks. Furthermore, we will explore strategic methods to accelerate the creation of functional solid-state materials with NCS properties.

## References

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