

#ICMolTalks

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📍 SS6



## Abstract

### ***Title: Ferroelectric polarization in antiferromagnets***

Ferroelectrics are fascinating materials that combine fundamental physics, with applications ranging from memory devices and sensors to energy harvesting and medical imaging. Since their discovery in the early 20th century, ferroelectrics have played a pivotal role in science and technology. In this talk, I will introduce the fundamental ideas of ferroelectricity, beginning with its brief historical development. In this talk we will also explore the different types of ferroelectrics displacive, order-disorder, proper, improper, hyperferroelectric highlighting their unique microscopic mechanisms and characteristic signatures. These conceptual foundations naturally lead to a discussion on lattice dynamics, where ferroelectricity can be understood as the “freezing” of specific phonon modes. Moving forward, I will discuss the microscopic origin of ferroelectricity, especially the role of lattice vibrations and soft phonon modes in driving the transition. Finally, I will present recent insights into the ferroelectric mechanism of Copper (II) hydroxide,  $\text{Cu}(\text{OH})_2$  as an illustrative case study, linking the conceptual foundations to current research. Through the first-principles studies and group theory analysis, we have provided a systematic theoretical investigation of vibrational properties in the hypothetical  $\text{Cmcm}$  high-symmetry phase to identify the symmetry-allowed ferroic phases. We identified a non-polar to polar ( $\text{Cmc}2_1$ ) phase transition, in which the displacive transformation is primarily responsible for the phase change induced by two  $B_{1u}$  (i.e.  $\Gamma_{-2}$ ) phonon modes within the centrosymmetric phase. The two polar structures have the same space group with different atomic arrangements. These structures correspond to different degrees of polarization (i.e.  $P_s = 3.06 \mu\text{C}\cdot\text{cm}^{-2}$  and  $P_s = 42.41 \mu\text{C}\cdot\text{cm}^{-2}$ ) with non-linear behavior under epitaxial strain, emerging from the parent high symmetry structure.