

Oral presentation

A soft phonon mode mechanism for chiral phase transitions in crystals**Eric Bousquet, Mauro Fava***University of Liège**eric.bousquet@uliege.be*

We demonstrate from first-principles calculations and symmetry analysis that a structural phase transition from an achiral to a chiral crystalline phase can be mediated by a soft phonon mode. This possibility is illustrated in the case of the K_3NiO_2 crystal, where an unstable and doubly degenerate zone boundary phonon mode is shown to lower the symmetry to a pair of enantiomorphic space groups. Examination of the related energy landscape shows that four degenerate domains can exist but described by two different space groups corresponding to the two enantiomorphic ones. We then explore how this structural chiral energy landscape is enhanced or reduced by pressure, strain or electric field. This allows us to explore strategies that could be used to induce an enantiomeric excess during the phase transition. At last we will discuss which of the known chiral crystals within enantiomorphic chiral space groups could have such a mechanism of displacive chiral phase transitions and how to find new candidates in inorganic periodic crystals as the number of known candidates is scarce.