Pressure mediated structural transition in $EuTiO_3$

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The phase competition in compounds with perovskite structure leads to phenomena related with a broad range of applications [1]. $EuTiO_3$ is an incipient ferroelectric with magnetic cations, thus it can potentially be used in information technology.
The phase purity and the lattice dynamics in bulk $EuTiO_3$ were investigated both microscopically, using X-ray and neutron diffraction, ^{151}Eu-Mössbauer spectroscopy, and ^{151}Eu nuclear inelastic scattering, and macroscopically using calorimetry, resonant ultrasound spectroscopy, and magnetometry at ambient pressure [2]. Lately, we carried out X-ray diffraction and ^{151}Eu nuclear forward scattering under externally applied pressure, up to 30 GPa. Our investigations were corroborated by *ab-initio* theoretical studies [3].
The perovskite symmetry, $Pm\bar{3}m$, is unstable at the *M*- and *R*-points of the Brillouin zone. The lattice instabilities are lifted when the structure relaxes in one of the symmetries: *I*4*/mcm*, *Imma*, $R\bar{3}c$ with relative relaxation energy around −25 meV. A stiffening on heating around room temperature is indicative of a phase transition similar to the one observed in $SrTiO_3$, however, although previous studies reported the structural phase transition to the tetragonal *I*4*/mcm* phase [4] our detailed sample purity analysis and thorough structural studies using complementary techniques did not confirm a direct phase transition. Instead, in the same temperature range, Eu delocalization is observed in line with our theoretical calculations. Furthermore, a pressure mediated structural transition to the *Imma* symmetry was found under 12 GPa applied pressure.

References

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