

The effect of pressure on the structure and dynamics of rutile phase dioxides

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The sequence of phase transition in ZrO_2 , TeO_2 , SnO_2 and RuO_2 has attracted a special attention in the field of crystal chemistry, earth science and materials science. The lack of an adequate behavior of rutile type SiO_2 , SnO_2 and RuO_2 motivated many theoretical and experimental studies to understand the phase transition and amorphisation under ambient and extreme conditions like high pressure. This rutile type phase undergoes structural phase transition under high pressure to the $CaCl_2$ type structure. Of particular interest for accurate prediction are where and whether phase transition occur, since these give rise to density discontinuities, which can account for known seismic effects or even after the convention patterns in the mantle. In the present study, we present the first principles study on lattice dynamics, Raman modes and phonon dispersion curves with high pressure for SnO_2 and RuO_2 in ferroelastic Rutile to $CaCl_2$ phase. The phase transition pressure from rutile to $CaCl_2$ structure obtained in the present study is in excellent agreement with experimental Raman, X-ray and Brillouin scattering data. The softening of the Raman active B_{1g} phonon mode, which is responsible for the structural phase transition, is demonstrated.

Biography

Prafulla K. Jha has been a fulltime Professor at Department of Physics, MK Bhavnagar University, Bhavnagar, India from September 2007. Prof. Jha is a theoretical condensed matter physicist with some overlap with experimental aspects. His research includes- First principles calculation of electronic structure and vibrational properties of complex solids, first principles and model calculation of vibrational properties of nanomaterials, Raman spectroscopy of nanomaterials and materials at high pressure. There are several recognitions to his credit that include ICTP, Trieste, Italy and TWAS associateship, UGC Research Award by University Grants Commission (UGC), New Delhi, young scientist award from the DST, Govt. of India. He has published more than 120 research papers in the referred reputed journals. He is member of the editorial board of quite a few journals. He has visited many international laboratories for academic purposes.

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