in the vicinity of the MPB [2]. The DFT code ABINIT [3] was used to compute the total energies, phonon frequencies and piezoelectric properties at different pressures.


Keywords: lead titanate, hydrostatic pressure, piezoelectricity

P08.06.53
Computational and experimental studies of the phase transitions of WO3
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Tungsten trioxide (WO3) exhibits several phase transitions below its melting point at 1700 K, summarized as: $PcZ=4 \rightarrow D P=1 Z=8 \rightarrow D P2_1/n Z=8 \rightarrow C Pbnm Z=4 \rightarrow C P4/nnc Z=2$ where $Z$ is the number of formula units per primitive cell. First order and continuous phase transitions are indicated by D and C, respectively. The phase transitions, from left to right, occur at around 230, 300, 623, 1070 and 1170 K, respectively [1]. Most of the transitions involve oxygen octahedral tilts, which are central for the phase transition mechanisms, since they allow the ratio between oxygen octahedral and cuboctahedral volumes to vary. The changes in bond lengths and angles correlate with the changes in electronic energy band structure: large changes in optical band gap and electrical resistivity occur at the $P1$ to ferroelectric $Pc$ phase transition [2], consistently with our density functional theory (DFT) computations. The ferroelectric distortion, spontaneous polarization and piezoelectric constants were estimated by DFT computations. The crystal size affects the phase transition temperatures and symmetries. We prepared small particle size WO3 powders to systematically study the size effects on the crystal symmetry and physical properties.


Keywords: tungsten trioxide, particle size, density functional theory

P08.06.54
Low-melting organic salts: A study of symmetry modification through phase transitions
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