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Pressure-induced anomalous enhancement of piezoelectricity and polarization rotation via an unexpected monoclinic phase of $PbTiO_3$[1] ZHIGANG WU, RONALD E. COHEN, Geophysical Lab, Carnegie Institution of Washington — Pressure-induced phase transitions and piezoelectricity of $PbTiO_3$ were studied using the *ab initio* density functional perturbation theory (ABINIT4.3.3). A tetragonal ($P4mm$) to monoclinic (Pm) phase transition occurs at 9 GPa, while this monoclinic phase transforms into paraelectric cubic phase at 22 GPa. The monoclinic (Pm) phase acts as the pressure-induced structural bridge between the tetragonal ($P4mm$) and rhombohedral ($R3m$) phases since its polarization rotates continuously in the pseudocubic ($\bar{1}10$) plane from the [001] towards the [111] pseudocubic directions. Under hydrostatic pressure, the enthalpy ($H = E + PV$) difference between the tetragonal and rhombohedral phases becomes tiny, and the polarization rotation via the monoclinic phase is possible, which results in huge enhancement of the piezelectric constant e_{15}, very similar to relaxor PZT. At 9 GPa, the spontaneous polarization is roughly half of that at 0 GPa, while the piezoelectric coefficient d_{15} is comparable in magnitude to d_{33} of relaxors PMN-PT and PZN-PT.

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