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Ferroelectricity in $PbTiO_3$ and $BaTiO_3$ under Pressure R.E. COHEN, Z. WU, Carnegie Institution of Washington — First-principles total energy and linear response calculations reveal a complicated pressure-induced phase transition sequence for $PbTiO_3$ (PT) under pressure. The previously proposed $P4mm$-to-Cm-to-$R3m$-to-$Pm\bar{3}m$ transition sequence [1] is not complete because only zone-center (Γ) instabilities and pressures P less than 30 GPa were considered. Recently Kornev *et al.* reported an unexpected enhancement of ferroelectric instability at high pressures [2]. Our computations confirm this result, and in addition, the zone-boundary R-point rotational instability is enhanced with pressure. Preliminary results show $R3m$-to-$R3c$-to-$R\bar{3}c$-to-$R3c$ phase transitions in PT for 18 GPa $< P <$ 120 GPa due to the competition and interaction of zone-center and zone-boundary instabilities. On the other hand, there is no instability in cubic $BaTiO_3$ for $P > 10$ GPa up to 120 GPa, resulting in a single $R3m$-to-$Pm\bar{3}m$ transition at 0 K. We are investigating whether the covalency of Pb is responsible for the unusual enhancement of ferroelectricity under high pressure. The electromechanical coupling constants become enormous in the transition regions from the tetragonal to high pressure phases for PT, suggesting that the large coupling in PT solid solutions such as PZT, PMN-PT, and PZN-PT, simply tune this transition to zero pressure[1]. Supported by ONR. [1] Z. Wu and R. E. Cohen, Phys. Rev. Lett. **95**, 037601 (2005). [2] Kornev *et al.*, Phys. Rev. Lett. **95**, 196804 (2005).

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