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Phase transition in BaThO₃ from *Pbnm* to *Ibmm* turn the fundamental energy band gap from indirect to direct

A.H. Reshak, Z.A. Alahmed, J. Bila

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- 1. The phase transition in BaTheO3 cause energy gap changes from indirect to direct.
- 2. The calculated energy gap is about 4.9 eV (Pbnm) and 4.6 eV (Ibmm)
- 3. The *Pbnm* and *Ibmm* phases exhibit negative uniaxial anisotropy and birefringence.
- 4. At room temperature BaThO₃ is stable in the *Pbnm* phase.
- 5. At room temperature BaThO₃ is stable in the *Ibmm* phase.

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