

Band Degeneracy in W-doped BaTiO₃: An Insight from Theoretical Approach with Experiment

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ABSTRACT

The structural, dielectric, and conduction mechanisms have been studied for BaTiO₃ (BTO) and BaTi_{0.85}W_{0.15}O₃ (BTWO) ceramics synthesized through the double sintering approach. X-ray diffraction (XRD) analysis confirms that both materials adopt a tetragonal perovskite structure (P4mm space group). Calculations based on Density Functional Theory (DFT) instruct perceptions into the electronic band structure and geometric optimization of the tetragonal segment, revealing an indirect bandgap with 3.28 eV and 2.21 eV for BTO and BTWO respectively, and demonstrating a remarkable transformation of a general n-type semiconductor to a p-type degenerate semiconductor. The Fermi level in BTWO shifts downward (1.64 to 1.15 eV) relative to BTO, as evidenced by fermi energy, the Moss-Burstein shift (2.11×10^{-4}), and charge carrier concentration calculations. Dielectric studies across 300-450 K display a clear ferroelectric-to-paraelectric phase transition in both materials. Notably, BTO reveals behavior between a typical ferroelectric and optimal relaxor, while BTWO is assessed as a canonical relaxor. Frequency-dependent resistivity (ρ_{ac}) measurements in addition elucidate the conduction mechanisms, contributing valuable insights into the dielectric and electronic properties of W-doped BaTiO₃ ceramics. Notably, this degenerate behavior will provide immense implications for the improvement of advanced substances for practical applications in electronics, thermoelectric devices, memory systems, and energy storage.

Keywords: Perovskite, Band degeneracy, Conduction Mechanism, Dielectric properties, Relaxor Ferroelectric.