Contribution ID: **149** Type: **Oral**

Mn-Doped $BaSnO_3$ Perovskites for Next-Generation Optoelectronics: A First-Principles Investigation

Thursday 6 November 2025 14:20 (15 minutes)

Perovskite oxides with the general formula ABO_3 offer highly tunable physical properties through substitution at the A and B lattice sites. In this work, manganese (Mn) was introduced into $BaSnO_3$ to evaluate its impact on structural, electronic, and optical properties. First-principles calculations were performed using density functional theory (DFT) within the pseudopotential plane-wave (PP-PW) framework implemented in Quantum Espresso for $BaSn_{1-x}Mn_xO_3$ (x = 0, 12.5, 25, and 37.5%). The lattice parameter decreases linearly with Mn incorporation, from 4.10 Å in pristine $BaSnO_3$ to 4.03 Å at x = 37.5%. The undoped compound exhibits a direct bandgap of 2.76 eV at the Γ point, which narrows significantly to 0.82 eV at 37.5% Mn doping due to enhanced Mn–O hybridization and altered orbital contributions within the valence band. Optical calculations reveal a progressive increase in the imaginary dielectric function $\varepsilon_2(\omega)$, with static values rising from 0.07 (x = 0) to 3.21 (x = 37.5). This trend leads to marked enhancement of absorption coefficients, from 2.68×10^5 to 6.23×10^5 cm^{-1} in the UV region and from 1.47×10^5 to 3.8×10^5 cm^{-1} in the visible range, accompanied by a decrease in optical transmittance from ˜80% to <76%. Overall, Mn doping enables precise tuning of the structural and optoelectronic response of $BaSnO_3$, underscoring its promise for advanced optoelectronic applications.

Type of presence

Presence online

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Session Classification: Perovskites & Semiconductor Devices (PV/LED)