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First-principles calculations to investigate the optical properties of ASnO3 (A = Ba, Ca, Sr, and Mg) perovskite oxides for the optoelectronic applications

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Advances in material engineering have demonstrated the high stability and low toxicity of tin-based perovskites, presenting an excellent lead-free alternative. Consequently, an ab initio study was conducted to investigate the structural, electronic, and optical properties of the tin-based perovskite oxides ASnO3 (A = Ba, Ca, Sr, Mg). The structural parameters showed highly consistent results with previous experimental and theoretical findings. The electronic calculations revealed semiconductor characteristics with indirect bandgaps. Analysis of the optical properties indicated significant absorption behaviour and weak reflection performance. Overall, these tin-based perovskite oxides hold great potential as materials for the electronic industry, particularly in optoelectronic applications.

Type of presence

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