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Sr_3SbI_3 Perovskite: First-Principles Insights into Radiation Tolerance, Ionic Dynamics, and Lattice Stability for Nuclear Applications

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Lead-free perovskites have emerged as pivotal materials for sustainable optoelectronics and radiation-resistant technologies. This study presents a comprehensive first-principles investigation of Sr_3PI_3, a novel perovskite, leveraging density functional theory (DFT) and molecular dynamics (MD) simulations via Quantum ESPRESSO to elucidate its electronic, structural, and dynamical properties. Self-consistent field (SCF) calculations achieved robust convergence with a total energy of −2477.04 Ry, validated by energy decomposition analysis. Band structure computations along a high-symmetry k-path revealed electronic dispersion characteristics, while preliminary density-of-states (DOS) analysis suggested a potential wide bandgap, necessitating further refinement. MD simulations under an NVT ensemble highlighted distinct ionic dynamics: iodine (I) exhibited notable mobility (displacements up to 0.1 Å), contrasting with the rigidity of antimony (Sb) and minimal strontium (Sr) displacements. BFGS relaxation confirmed structural stability, with forces converging below 1.0×10^{-3} Ry/au.

The material's dual behavior—combining a stable Sb-Sr lattice framework with mobile iodine sublattices—positions it as a promising candidate for nuclear applications. Sb's immobility may enhance radiation tolerance by mitigating defect formation, while iodine's diffusivity suggests potential self-healing mechanisms under irradiation. These attributes align with requirements for neutron moderation and shielding materials, where structural integrity and controlled ionic transport are critical. Additionally, the electronic structure insights lay groundwork for radiation-tolerant semiconductor devices.

Future work will refine DOS resolution, probe high-temperature MD behavior, and simulate radiation damage to directly assess defect dynamics. This study establishes Sr_3PI_3 as a compelling platform for advancing both condensed matter physics and nuclear materials engineering, bridging atomic-scale properties to macroscopic performance in extreme environments.

Keywords: Lead-free perovskite, first-principles simulations, radiation tolerance, ionic

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