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Synergistic Effects of Intrinsic Defects and Material Composition on the Scintillation Properties of Bismuth-Based Scintillators

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We conduct a comprehensive analysis of the structural, electronic, and optical properties of bismuth-based scintillators, with a particular focus on the role of intrinsic defects and material composition.
We employ density functional theory (DFT) calculations with the PBE0 hybrid functional, we delve into the nuances of defect processes in Bi4Ge3Si3O12 (BGO) scintillators and explore the influence of varying Ge/Si ratios in Bi4Ge3xSi3(1-x)O12 (BGSO) crystals. Our investigation reveals that intrinsic defects, particularly antisite types, significantly influence the scintillation performance by introducing ingap states and affecting charge trapping mechanisms.

Field

Detectors and electronics

Primary authors: BOUHALI, Othmane (Texas A&M University at Qatar); Dr OMOTAYO, Salawu (Texas A&M)

Presenter: BOUHALI, Othmane (Texas A&M University at Qatar)

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