

Abstract Submitted
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Comparative study of electronic structures and nonproportionality of scintillator materials¹ WAHYU SETYAWAN, Duke University, ROMAIN GAUME, ROBERT FEIGELSON, Stanford University, STEFANO CURTAROLO, Duke University — The electronic structures of selected scintillator materials for gamma-ray detection are calculated. We use Vienna Ab-initio Simulation Package with projector augmented waves pseudopotentials and exchange-correlation functionals as parameterized by Perdew-Burke-Ernzerhof. Curvatures of the top of valence band and the bottom of conduction band are calculated. Parameters are introduced to measure the degree of nonproportionality of photon response of the scintillators. The data show an interesting correlation between the band curvatures and the nonlinearity. The results can be used to guide the design of future proportional scintillators.

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Wahyu Setyawan
Duke University

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