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Defect process in BGO: A precursor to band-edge engineering and design of stable scintillators

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Scintillating materials suffer degradation while in operation due to defects induced in the process. Lattice defects could severely impact detector efficiency via non-radiative transfer of electron excitation. Like most materials for this kind of applications, there is a strong performance-structure relationship. An understanding of the defect formation process is therefore important in the design of resilient scintillators. Bismuth germanate Bi4 Ge3 O12 (BGO) has been extensively studied as a luminescent material that emits light in the visible region upon exposure to ionizing radiation. Investigating the likelihood of band gap engineering (BGE) in bismuth germanate considering trap depths of intrinsic defects is essential for improving existing materials and in the design of new ones. In this work, using density functional theory, we studied the formation energies of vacancies/interstitials, cation antisites in pristine BGO. To provide insights into factors affecting the stability of doped systems and unravel the origin of the activity of doped BGO, we investigate the structural properties, energetics of pristine and REE (Nd, Pr, Ce and Tm) doped BGO using first principles methods. We reproduced the band gap of the pristine BGO to within experimental reported value using the hybrid PBE0 functional. Analysis of defect energetics reveals a strong dependence of properties on defect types. Further investigations lead to the discovery of energy levels induced by the defects providing a route for the possibility of manipulating the electronic properties for target application. It provides an understanding of ways that could be adopted to suppress hot electron thermalization that could lead to intra-band luminescence of charge carriers. Our analysis of the role of doping on BGO confirms route for the modification of the stability of the system in presence of defects. Analysis of the optical properties reveals variations in different regions of photon energy spectra.

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