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

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Introduction and Motivation

- **Defects and Composition Analysis:**Exploration of intrinsic defects in cation doped (BGO) using Density Functional Theory (DFT) with PBE0 hybrid functional.
- **Defect Dynamics and Scintillation Performance:** Quantitative analysis of defect formation energies and their influence on charge trapping and ingap states, essential for understanding scintillation responses.
- **Doping Effects and Material Variations:** Studying rare earth elements (REE) doping impacts and compositional changes in BGO systems to uncover interactions affecting electronic structures and scintillation properties.

Methodology

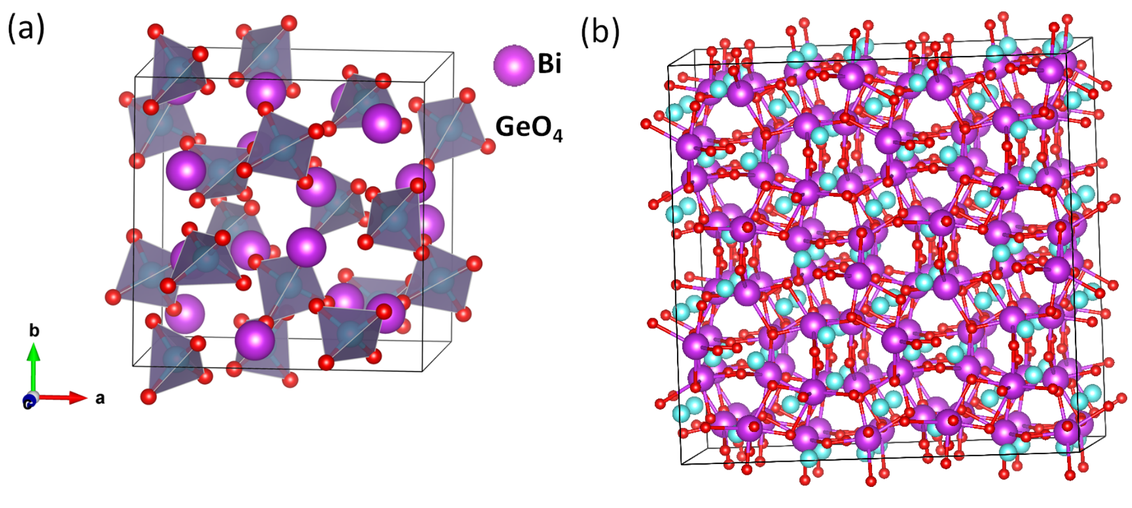

Figure 1. (a) Crystal structure of optimized BGO unit cell and (b) 2×2×2 supercell used for defect simulations

- Employed DFT with PBE0 hybrid functional to assess structural and electronic impacts in BGO and REE-doped BGO.
- Simulated various defect types to evaluate formation energies and influence on electronic properties.
- Examined effects of rare earth doping on BGO, focusing on formation energies and oxygen vacancy formation.

Results: Structural and Electronic Properties

Structural Properties:

- Analysis of the lattice constants, bond lengths and band gap in BGO
- Calculated lattice parameters and the band gaps of pristine BGO

	Our work	Exp [2]	previous theory [3]
Bi-O	2.15Å	2.14Å	2.20Å
	2.63 Å	2.61Å	2.62Å
Ge-O	1.75Å	1.74Å	1.76Å
Band gap	3.4 eV	4.7 eV	3.5
	4.6 eV		

- Obtained values are in agreement with previous work
- **Electronic properties of pristine BGO:** Pristine BGO exhibits a wide indirect band gap which is crucial for its application in scintillation

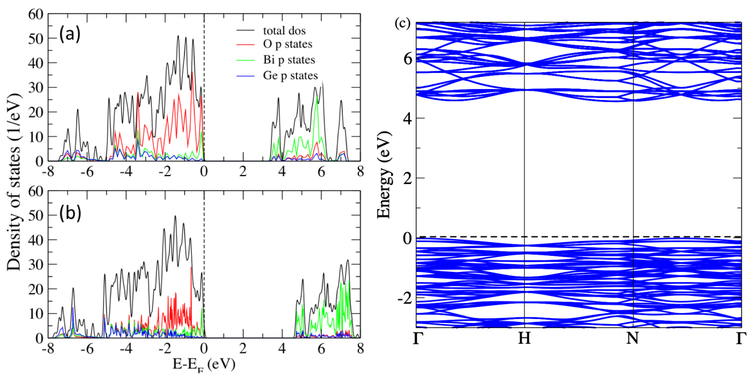

Figure 2. Total and partial density of states BGO calculated using (a) DFT-GGA (b) DFT-PBE0 and (c) band structure of pristine BGO

Results: Effect of defects on properties

- **Formation eneretics of intrinsic defect** Intrinsic defects in BGO, like vacancies and interstitials, form during crystal growth or irradiation, affecting its electronic and optical properties.

Table 1. Formation energies of intrinsic defect

Defect type	Formation energy (eV)
O vacancy	2.30 (2.32)
Ge vacancy	7.33
Bi vacancy	3.61
O interstitial	3.26 (3.28)
Bi interstitial	5.70

- Oxygen vacancies, with the lowest formation energy at 2.30 eV, are most likely to form, while germanium vacancies and bismuth interstitials, with higher energies, are less probable
- Effect of defects on electronic properties
- creation of ingap states, affecting charge trapping, thereby impacting scintillation performance.

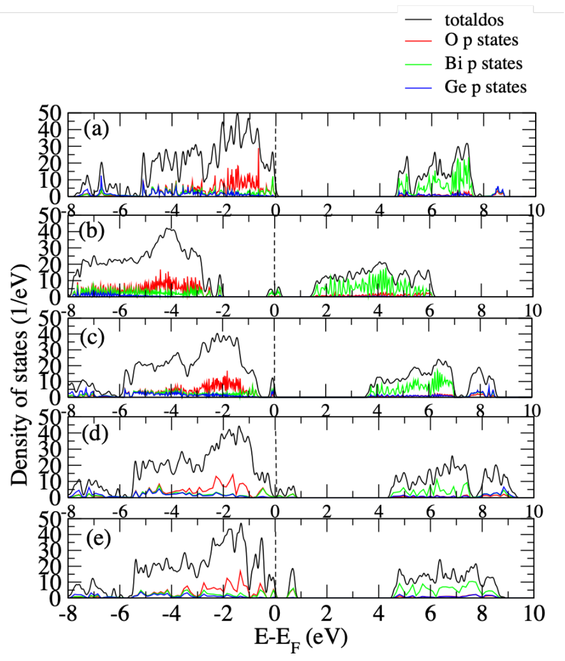

Figure 3. Total and partial density of states of (a) pristine BGO and BGO (b) antisite defect (c) O vacancy defect (d) Bi vacancy defect (e) Ge vacancy defect.

Optical absorption spectra.

- Assessed the optical absorption and emission properties, correlating structural and electronic changes with optical behavior.

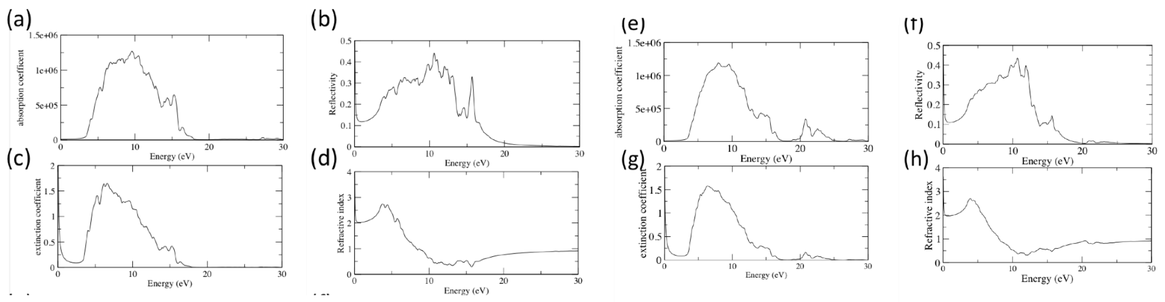

Figure 4. The calculated of (a) absorption coefficient (b) reflectivity, (c) extinction coefficient and (d) refractive index of pristine BGO.Right panel presents (d) absorption coefficient (e) reflectivity, (f) extinction coefficient and (g) refractive index of Ce-doped BGO.

Conclusion

- Our DFT studies suggest that controlling specific defects could tailor properties of BGO for improved performance in radiation detection.

Acknowledgments

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