

ORIGINAL ARTICLE

Dielectric and electronic structure modulation in andalusite through nitrogen and boron substitution: a first-principles study

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ABSTRACT – The dielectric and electronic properties of Al_2SiO_5 were studied using density functional theory (DFT) with the GGA PBE and meta-GGA $r^2\text{SCAN}$ functionals. The orthorhombic andalusite structure was optimized with each functional. Compared with PBE, $r^2\text{SCAN}$ gave lattice parameters closer to the experimental values and a larger band gap, and was therefore used to examine the substituted structures. Boron and nitrogen were introduced by replacing Al and O, respectively, while P substitution at the Si site was included for comparison. The PDOS of pristine andalusite shows a valence band dominated by O-2p states, with contributions from Al and Si near the conduction-band edge. Both B1 and B2 remained insulating after substitution, with B-O hybridization appearing in the valence band region. In contrast, N and P substitution produced states near the Fermi level. The charge-density-difference maps also show that the distribution of charge depends on the substitution site. B1 shows a more localized redistribution around the B-O region, whereas B2, N, and P produce more anisotropic redistribution. For the insulating B-substituted systems, the dielectric response increased slightly relative to pristine andalusite, accompanied by changes in the refractive index and absorption spectra. These findings indicate that the electronic and dielectric properties of andalusite depend on both the substituting element and its local coordination environment.

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INTRODUCTION

Aluminium silicate (Al_2SiO_5) is an important oxide material that combines alumina and silica structural units within a single crystalline structure. The material exhibits high thermal stability, low intrinsic electrical conductivity, and good chemical resistance, making aluminosilicate systems relevant for refractory ceramics, dielectric materials, catalyst supports, and insulating oxide applications [1–3]. Al_2SiO_5 exists in three polymorphs, namely andalusite, sillimanite, and kyanite, which are stabilized under different temperature and pressure conditions [4–6]. Although these polymorphs possess identical chemical composition, their local atomic coordination environments differ significantly, resulting in distinct bonding characteristics, lattice distortions, and electronic distributions within the Al-O-Si structure [7,8].

Among the Al_2SiO_5 polymorphs, andalusite provides a suitable structural model for investigating substitution-induced electronic modulation because of its relatively stable orthorhombic structure and moderate structural complexity. The andalusite structure consists of interconnected Al-O and Si-O polyhedral that generate anisotropic bonding environments while maintaining lower structural density compared with kyanite [9,10]. The periodic structure also permits substitution at different atomic sites while retaining the andalusite structure, allowing the effects on electronic, dielectric, and optical properties to be compared. In addition, the wide-gap insulating nature of aluminosilicate systems makes andalusite attractive for studying dielectric-property modulation through controlled substitutional engineering.

Density functional theory (DFT) provides an effective method for investigating these phenomena at the atomic scale through direct evaluation of electronic density, total energy, and interatomic interactions without empirical fitting parameters [11]. Previous theoretical and spectroscopic studies demonstrated that the electronic structure of Al_2SiO_5 polymorphs is strongly dominated by hybridization between O-2p, Al, and Si electronic states [12,13]. Experimental X-ray photoelectron spectroscopy (XPS) and electron energy-loss spectroscopy analyses further showed that the upper valence-band region mainly originates from O(2p)-dominated hybridized orbitals distributed throughout the aluminosilicate structure [14]. Accurate description of this electronic redistribution is therefore important for understanding polarization behavior and substitution-induced modification of dielectric and optical properties.

Conventional local-density approximation (LDA) and generalized-gradient approximation (GGA) functionals often underestimate band gaps and excessively delocalize electronic density in insulating oxide systems. These limitations can affect prediction of dielectric response and optical transitions, particularly in mixed ionic and covalent oxide structure such as aluminosilicates. Meta-GGA approaches provide improved treatment of intermediate range electronic correlation while maintaining efficient computational cost. In particular, the regularized strongly constrained and appropriately normed functional (r^2 SCAN) developed by Furness et al. improves the numerical stability of the original SCAN formalism while preserving accurate prediction of structural and energetic properties [15]. Previous benchmark studies reported that r^2 SCAN improves lattice-parameter and electronic-property prediction for oxide materials relative to conventional GGA approaches [16,17]. This balance between structural accuracy and numerical stability makes r^2 SCAN suitable for investigating dielectric and optical behavior in aluminosilicate systems.

In addition to ground-state electronic analysis, frequency-dependent dielectric calculations provide important information regarding electronic polarization, dielectric screening, interband transitions, and optical response. The real dielectric component $\epsilon_1(\omega)$ and imaginary dielectric component $\epsilon_2(\omega)$ allow direct correlation between microscopic electronic redistribution and macroscopic dielectric behavior. Refractive index and absorption coefficient can also be derived from the dielectric spectra, enabling evaluation of substitution-induced modification of optical properties. Combined with projected density-of-states (PDOS) and charge-density-difference analyses, this approach enables detailed interpretation of local electronic modulation within the substituted aluminosilicate structure.

In this work, the andalusite phase of Al_2SiO_5 was used as a structural model to investigate how light-element substitution modifies dielectric and electronic behavior. Boron substitution at the Al site ($\text{B} \rightarrow \text{Al}$) and nitrogen substitution at the O site ($\text{N} \rightarrow \text{O}$) were selected as representative cationic and anionic substitutions, respectively. Phosphorus substitution at the Si site ($\text{P} \rightarrow \text{Si}$) was also considered to examine the influence of tetrahedral-structure distortion on the electronic structure. The effects of these substitutions on structural stability, electronic states, charge redistribution, dielectric response, and optical properties were analyzed using DFT calculations based on the PBE and r^2 SCAN functionals. This study provides microscopic insight into substitution-induced electronic modulation in aluminosilicate structure and demonstrates the potential of local substitutional engineering for tuning dielectric and optical properties of functional oxide materials.

METHODOLOGY

All first-principles calculations were performed using Quantum ESPRESSO version 7.5 [18,19] within the density functional theory (DFT) framework. The plane-wave pseudopotential method was applied using scalar-relativistic PAW-type pseudopotentials for Al, Si, O, B, N, and P atoms. Exchange–correlation interactions were described using the LDA-PZ, GGA-PBE, and meta-GGA r^2 SCAN functionals with consistent pseudopotential sets for each functional level. The initial Al_2SiO_5 structure was constructed from the experimental CIF data (COD 1010924) with orthorhombic Pnnm symmetry (No. 58), followed by construction of a $1 \times 1 \times 2$ supercell for substitutional calculations.

Structural optimizations were carried out using plane-wave and charge-density cutoffs of 90 Ry and 720 Ry, respectively. A $3 \times 3 \times 2$ Monkhorst–Pack k-point grid was employed for structural optimization, while a denser $6 \times 6 \times 4$ k-point grid was used for electronic density-of-states and optical-property calculations. The total energy and force convergence thresholds were set to 10^{-5} Ry and 10^{-4} Ry Bohr $^{-1}$, respectively. Optimized lattice parameters obtained from the LDA, PBE, and r^2 SCAN functionals were compared with experimental structural data to evaluate the accuracy of each exchange–correlation treatment.

Substitutional models were generated by replacing selected atoms within the optimized andalusite supercell. Boron substitution was introduced at the two distinct Al coordination environments, with B1 corresponding to the six-coordinated octahedral Al[6] site and B2 to the five-coordinated Al[5] site. Nitrogen substitution was introduced at three nonequivalent oxygen sites, denoted as N1, N2, and N3. N1 corresponds to an O site coordinated to three Al atoms, whereas N2 and N3 correspond to distinct O sites each coordinated to one Si and two Al atoms. For comparison, phosphorus substitution at the four-coordinated tetrahedral Si[4] site was also evaluated and denoted as P1. The structural model and substitutional sites used in this study are illustrated in Figure 1. All substituted structures were fully optimized using the same computational parameters as the pristine system and subsequently analyzed using the r^2 SCAN functional to maintain methodological consistency for electronic and dielectric analysis.

Electronic structures were evaluated through projected density-of-states (PDOS) calculations to examine the contribution of individual atomic orbitals near the valence- and conduction-band regions. Charge-density-difference distributions were additionally calculated to evaluate local electronic redistribution induced by substitution

$$\Delta\rho = \rho_{\text{doped}} - \rho_{\text{pristine}} \quad (1)$$

where ρ_{doped} and ρ_{pristine} represent the charge densities of the substituted and pristine systems, respectively. Positive and negative isosurfaces correspond to charge accumulation and charge depletion regions.

Frequency-dependent dielectric properties were calculated from the electronic states obtained from the nonself-consistent calculation using a $6 \times 6 \times 4$ mesh. The frequency-dependent complex dielectric function was evaluated using the epsilon.x post-processing code of Quantum ESPRESSO within the independent-particle random phase approximation. The real, $\epsilon_1(\omega)$, and imaginary, $\epsilon_2(\omega)$, components of the dielectric function were calculated from the interband

electronic transitions. The static electronic dielectric constant was estimated from the low frequency limit, $\epsilon_1(\omega \rightarrow 0)$. The refractive index, $n(\omega)$, and absorption coefficient, $\alpha(\omega)$, were subsequently derived from the calculated complex dielectric function.

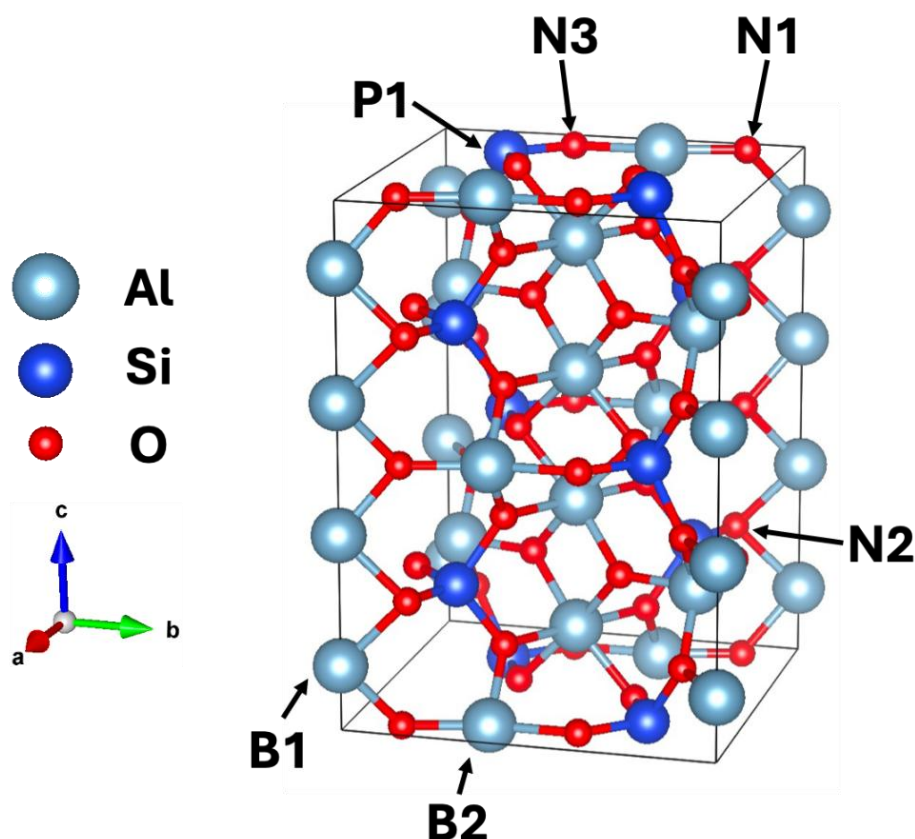


Figure 1. Structural model of the Al_2SiO_5 supercell used for substitutional calculations. B1 and B2 indicate substitution at the six-coordinated Al[6] and five-coordinated Al[5] sites, respectively. N1 indicates substitution at an O site coordinated to three Al atoms, whereas N2 and N3 represent two nonequivalent O sites coordinated to one Si and two Al atoms. P1 indicates substitution at the tetrahedral Si[4] site. The figure represents the initial structural model prior to structural optimization

RESULT AND DISCUSSION

The orthorhombic Al_2SiO_5 structure was optimized using the LDA, PBE, and $r^2\text{SCAN}$ exchange–correlation functionals. The calculated lattice parameters, unit-cell volumes, and band gaps are summarized in Table 1 together with experimental low-temperature structural data [20]. All functionals reproduced the andalusite structure without instability. Among the tested approaches, LDA produced the smallest average lattice-parameter deviation from experiment (0.64%), followed by $r^2\text{SCAN}$ (1.09%) and PBE (1.24%). Although LDA therefore provides the closest structural agreement, $r^2\text{SCAN}$ improves the structural prediction relative to PBE while providing a larger band gap. The calculated band gaps of 4.67, 4.53, and 5.69 eV obtained using LDA, PBE, and $r^2\text{SCAN}$ correspond to absolute deviations of 4.43, 4.57, and 3.41 eV, respectively, from the experimental value of 9.10 eV. Therefore, $r^2\text{SCAN}$ was selected for the subsequent calculations as a compromise between structural agreement and electronic-structure description [21–23].

Table 1. Calculated lattice parameters, unit-cell volume, and band gap of pristine andalusite obtained using LDA, PBE, and $r^2\text{SCAN}$ functionals compared with experimental data.

Functional	a-axis (Å)	b-axis (Å)	c-axis (Å)	Volume (Å ³)	Deviation (%)	Band gap (eV)
Exp. (10 K)	7.781	7.890	11.111	682.128	-	9.10
LDA	7.715	7.841	11.061	668.877	0.64	4.67
PBE	7.886	7.987	11.239	707.985	1.24	4.53
$r^2\text{SCAN}$	7.619	7.840	11.048	659.974	1.09	5.69

The optimized structural parameters of the substituted systems are summarized in Table 2. Boron substitution at the Al site produced slight lattice contraction due to the smaller atomic radius of boron relative to aluminum. The B1 and B2 configurations preserved insulating behavior with calculated band gaps of 5.27 and 5.19 eV, respectively. In contrast, all N-substituted configurations exhibited finite states near the Fermi level. The P1 configuration also exhibited metallic-like near-Fermi states following substitution at the tetrahedral Si site. These results indicate that the resulting electronic

behavior strongly depends on the local substitutional environment and coordination geometry within the Al–O–Si structure.

Table 2. Optimized structural parameters, total energies, and electronic characteristics of substitutional B-, N-, and P-doped andalusite configurations calculated using r^2 SCAN functional.

System	Energy (ry)	a-axis (Å)	b-axis (Å)	c-axis (Å)	Volume (Å ³)	Band gap (eV)	Substitution site
B1	-1419.30	7.6240	7.8187	10.9814	654.5956	5.27	Al[6] octahedral
B2	-1419.43	7.6053	7.8755	10.9426	655.4043	5.19	Al[5] (5-coordinated)
N1	-1405.72	7.6230	7.8470	11.0709	662.2324	-	O(3Al)
N2	-1405.73	7.6120	7.8527	11.0799	662.2989	-	O(1Si, 2Al)
N3	-1405.71	7.6401	7.8429	11.0502	662.1366	-	O(1Si, 2Al)
P1	-1422.89	7.6429	7.8308	11.0850	663.4086	-	Si[4] (tetrahedral)

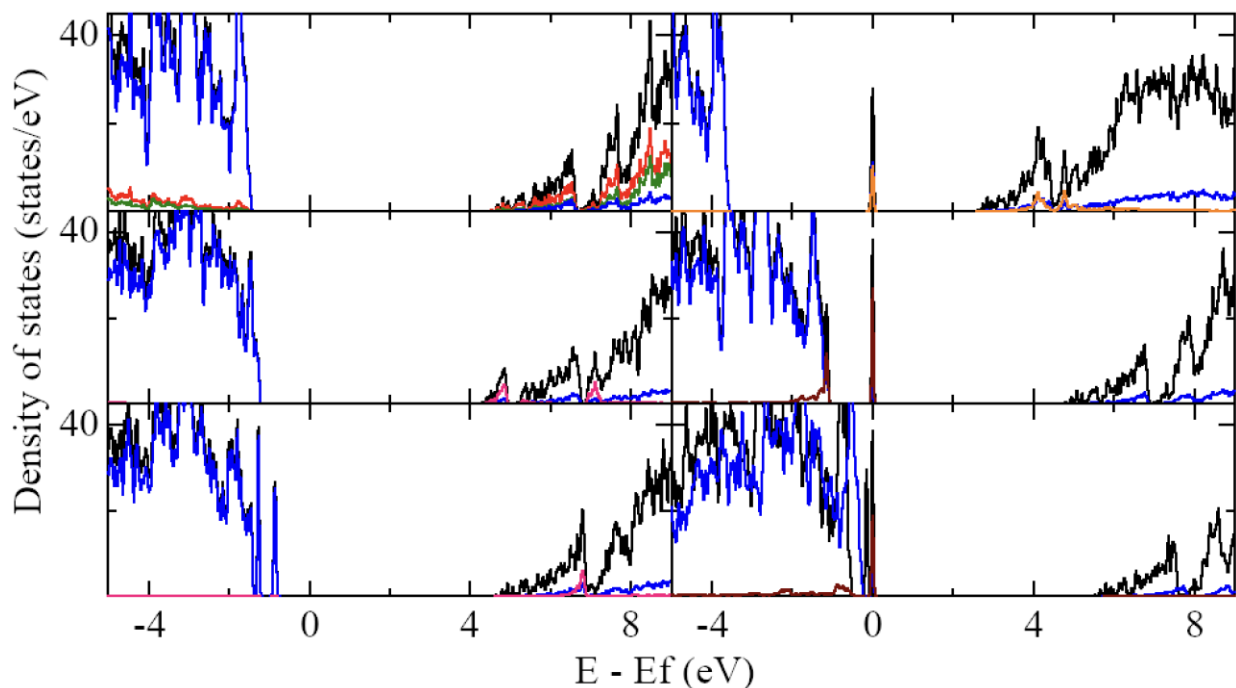


Figure 2. Projected density of states (PDOS) of pristine and substituted andalusite calculated using the r^2 SCAN functional. Left panels correspond to pristine and B-substituted systems, while right panels correspond to P- and N-substituted systems. The top-left panel shows pristine andalusite, where black, red, green, and blue curves represent total DOS, Al states, Si states, and O-p states, respectively. The middle-left and bottom-left panels show B1 and B2 configurations, respectively, where the magenta curves represent B states and the blue curves represent O-p states. The top-right panel corresponds to the P1 configuration, where the orange curve represents P states. The middle-right and bottom-right panels correspond to N1 and N2 configurations, respectively, where the brown curves represent N states. Black curves in all panels represent the total density of states

The projected density-of-states (PDOS) distributions calculated using the r^2 SCAN functional are shown in Figure 2. The pristine structure exhibits insulating behavior, with the valence band region dominated by O-2p states and smaller Al and Si contributions, while the conduction band edge consists of hybridized Al and Si states. For the B1 and B2 configurations, additional B states appear in the valence band region, indicating hybridization between B and neighboring O states. Since B and Al have the same oxidation state (+3), substitution of B at the Al site does not introduce an additional electron or hole, consistent with the insulating behavior of both B1 and B2. In contrast, substitution of N at the O site and P at the Si site changes the local electron count because N and O, and P and Si, have different valence states. In the present neutral supercells without additional charge compensating defects, these substitutions result in partially occupied states near the Fermi level. The N-substituted configurations show hole states, whereas P substitution introduces electron-donor states, consistent with the PDOS distributions shown in Figure 2.

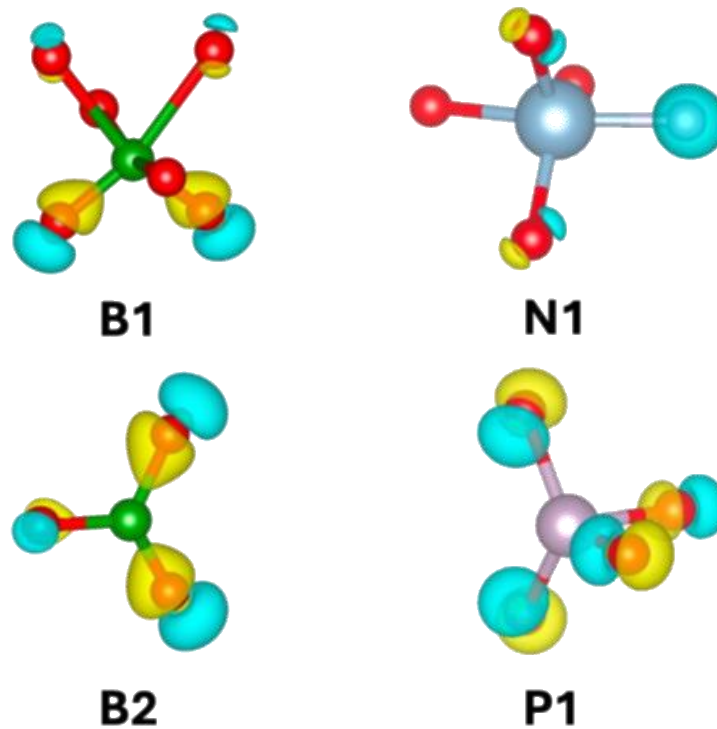


Figure 3. Charge density difference distributions of substituted andalusite structures calculated using the r^2 SCAN functional for B1, N1, B2, and P1 configurations. Yellow and cyan isosurfaces represent charge accumulation and charge depletion regions, respectively. Isosurface values of $\pm 0.15 \text{ e}/\text{\AA}^3$ were used for B1, B2, and P1, while $\pm 0.075 \text{ e}/\text{\AA}^3$ was used for the N1 configuration.

Charge-density-difference distributions for the substituted systems are presented in Figure 3. The B1 configuration shows charge accumulation and depletion concentrated around the substituted B-O coordination region. B2 shows a more directional redistribution along the B-O bonds. For N1, the redistribution is asymmetric around the substituted site, whereas P1 produces a broader redistribution around the tetrahedral region. These differences show that the spatial distribution of charge depends on the substitution site and its local coordination.

Table 3. Calculated dielectric properties of pristine and substituted andalusite obtained from the frequency-dependent dielectric function using the r^2 SCAN functional.

System	$\epsilon_{xx}(0)$	$\epsilon_{yy}(0)$	$\epsilon_{zz}(0)$	$\epsilon_{avg}(0)$	Transition onset (eV)
Pristine	2.5172	2.4435	2.4765	2.4791	6.17
B1	2.5596	2.4918	2.5349	2.5288	5.81
B2	2.5290	2.4590	2.4917	2.4933	6.10

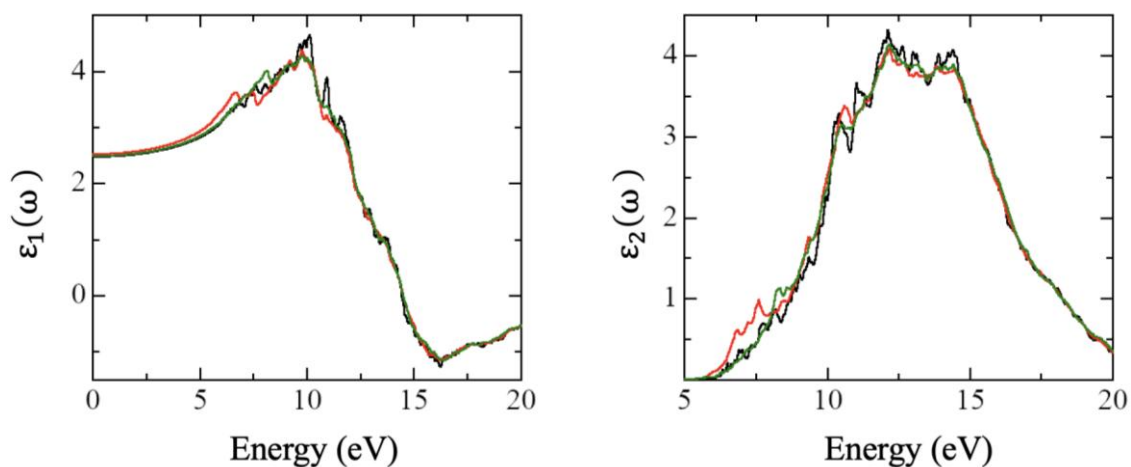


Figure 4. Frequency-dependent dielectric spectra of pristine and substituted andalusite calculated using the r^2 SCAN functional. The black solid line represents pristine andalusite, while the red and green lines correspond to the B1- and B2-doped systems, respectively.

The calculated dielectric properties are summarized in Table 3, while the frequency-dependent dielectric spectra are shown in Figure 4. Only the insulating pristine, B1, and B2 configurations were included in the dielectric and optical analyses. The N- and P-substituted systems were excluded because they exhibit partially occupied states at the Fermi level, for which the intraband contribution would need to be considered in addition to the interband transitions included in the present calculations. The pristine andalusite structure exhibits an average static dielectric constant $\epsilon_{\text{avg}}(0)$ of 2.4791. The average static dielectric constant increases from 2.4791 for pristine andalusite to 2.5288 for B1 and 2.4933 for B2, with B1 showing the largest increase. The real dielectric component $\epsilon_1(\omega)$ shows moderate enhancement within the intermediate-energy region for the substituted systems relative to pristine andalusite. Similarly, the imaginary dielectric component $\epsilon_2(\omega)$ exhibits small modifications in transition intensity and spectral shape following substitution. The earlier transition onset observed for B1 compared with pristine andalusite is consistent with the slight reduction of the calculated band gap and enhanced B–O hybridization observed in the PDOS analysis.

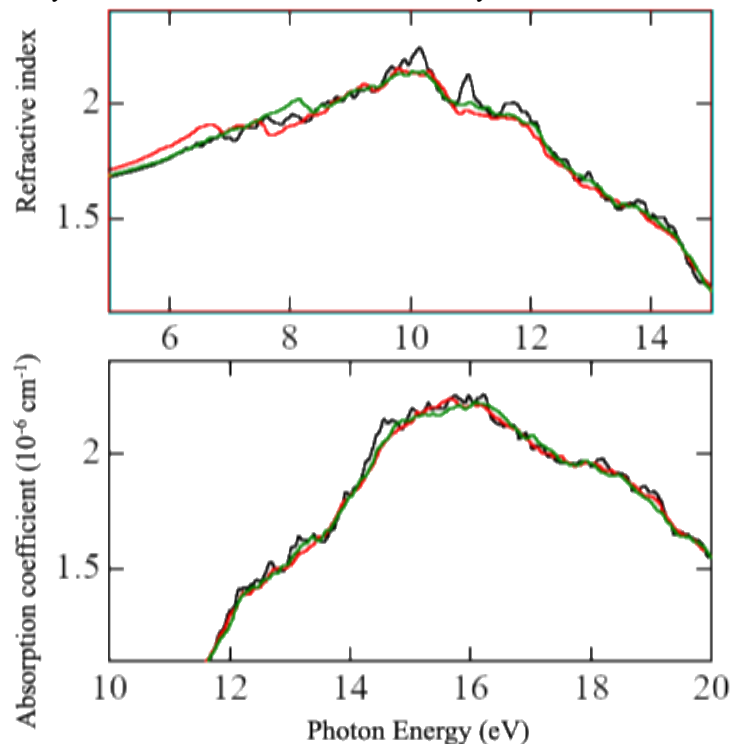


Figure 5. Optical properties of pristine and B-substituted andalusite calculated using the r^2 SCAN functional. Black, red, and green lines represent pristine, B1-, and B2-substituted configurations, respectively.

The optical properties derived from the dielectric spectra are shown in Figure 5. The refractive-index spectra, $n(\omega)$, exhibit similar overall spectral profiles for pristine and B-substituted systems, although slight differences appear within the low- and intermediate-energy regions. The B1 configuration shows slightly enhanced refractive response below approximately 8 eV, while the B2 configuration produces broader modification near the main spectral maximum around 9–11 eV. The absorption-coefficient spectra, $\alpha(\omega)$, additionally show small shifts in the absorption profile and transition intensity following substitution. The substituted systems exhibit slightly earlier absorption onset and modified spectral broadening relative to pristine andalusite, consistent with substitution-induced modification of the electronic states near the valence-band edge. Overall, the dielectric and optical analyses demonstrate that boron substitution can moderately tune the polarization and optical response of andalusite through modification of the local electronic structure and bonding environment [24,25].

CONCLUSION

The present study examined the effects of B, N, and P substitution on the electronic and dielectric properties of andalusite Al_2SiO_5 using DFT calculations. Among the considered functionals, LDA gave the smallest lattice-parameter deviation from experiment (0.64%), while r^2 SCAN gave a deviation of 1.09% and a band gap of 5.69 eV, closer to the experimental value of 9.10 eV than the LDA and PBE results. Based on this balance between structural and electronic description, r^2 SCAN was used for the substitutional calculations. B substitution at both the six-coordinated Al[6] and five-coordinated Al[5] sites preserved the insulating character, with band gaps of 5.27 and 5.19 eV for B1 and B2, respectively. In contrast, N substitution at the O sites and P substitution at the Si site produced partially occupied states near the Fermi level. The N-substituted systems showed hole states, whereas P substitution introduced electron-donor states. Charge density difference analysis showed that the redistribution of charge depends on the substitution site and its local coordination. For the insulating systems, B substitution increased the average static dielectric constant from 2.4791 for pristine andalusite to 2.5288 for B1 and 2.4933 for B2, accompanied by changes in the dielectric and optical spectra.

These results show that the substitution site and local coordination play an important role in determining the electronic and dielectric response of andalusite.

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