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First-principles investigation for some physical properties of some fluoroperovskites compounds ABF_3 (A = K, Na; B = Mg, Zn)

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Abstract: In this work, the structural, electronic and optical properties of fluoroperovskite ABF_3 (A = K, Na; B = Mg, Zn) were studied using two different approaches: the full-potential linearized augmented plane wave method and the pseudo-potential plane wave scheme in the frame of generalized gradient approximation features such as the lattice constant, bulk modulus and its pressure derivative are reported. The ground state properties of these compounds such as the equilibrium lattice constant and the bulk modulus are in good agreement with the experimental results. The first principles calculations were performed to study the electronic structures of ABF_3(A = K, Na; B = Mg, Zn) compounds and the results indicated that these four compounds are indirect band gap insulators. The optical properties are analysed and the source of some peaks in the spectra is discussed. Besides, the dielectric function, refractive index and extinction coefficient for radiation up to 25 eV have also been reported and discussed.

Keywords: Fluoroperovskite; FP-LAPW; PP-PW; Electronic structure; Optical properties

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1. Introduction

Numerous investigations have been extensively done regarding the cubic perovskites with different compositions and structures, motivated by their possible applications in numerous industrial and engineering domains [1–4]. They have shown a wide range of attractive properties ferroelectricity [5, 6], piezoelectricity [7, 8], semiconductivity [9], catalytic activity [10], thermoelectricity [11], superconductivity and metal–insulator transition [12]. As an example ternary oxides of rare earth (Eu, Gd, Tb)CoO_3 type oxides, this series reveal extensive applications in materials science and technology, some of the perovskites (Eu, Gd, Tb)CoO_3 compounds are used as electrode materials for magneto hydrodynamic (MHD)generators [13], for fuel cells [14], half-metallic [15]. On the other hand, perovskites like $BaMnO_3$ and $SrMnO_3$have attracted interest in NO removal process as catalysts [16–18]. Earlier works [19, 20] performed on oxide and semiconductor systems showed that the thickness of the metal slab becomes important in determining the electronic structure. A surface energy is converged quickly with increasing number of atomic layers.

Complex fluorides have unique characteristics in opto-electronic, and luminescent properties and also show various interesting structures [21, 22]. Among them, especially ternary fluorides with perovskite structure, KXF_3(X = Mg, Ca, Mn, Fe, Co, Ni, and Zn), have been in the limelight in these days and have been actively researched due to their high-temperature super-ionic behavior and physical properties, such as piezoelectric characteristics, ferromagnetic, antiferromagnetic, non-magnetic insulator behavior and so on [23–27]. Darabont et al. [28] investigated the $KMgF_3$ single crystals by X-ray diffraction and suggested that these crystals have a cubic perovskite

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*Corresponding author, E-mail: berrisaadi12@yahoo.fr structure with one molecule per unit cell, with lattice parameter a = 3.978 ± 0.05Å. The structures and phase transitions in the solid solution $Na_{1-x}K_xMgF_3$have been investigated recently by Zhao [29] and by Chakhmouradian et et al. [30]. Basically, $NaMgF_3$ perovskite was first synthesized by Ludekens and Welch [31] before natural $NaMgF_3$ was discovered by Chao et al. [32], where several experimental and theoretical studies have been reported [30, 33–36]. Generally,perovskites crystallize in orthorhombic structure, but many studies havede picted the cubic one [37–42].

The considered ABF_3 (A = K, Na; B = Mg, Zn) are presumed to have ideal cubic perovskite structure(#221) The cubic unit cell contains one molecule with the Wychoff positions of the atoms are A 1a (0, 0, 0), B 1b (0.5, 0.5, 0.5) and F 3c (0.5, 0.5, 0) In the present paper, the structural, electronic and optic forABF_3(A = K, Na; B = Mg, Zn) compounds are reported. The aim of this work is to examine the electronic band structure of ABF_3 (A = K, Na; B = Mg, Zn) with emphasis on its derived properties.

The calculations are performed using Full-relativistic (FP-LAPW) and the norm-conserving pseudo potential

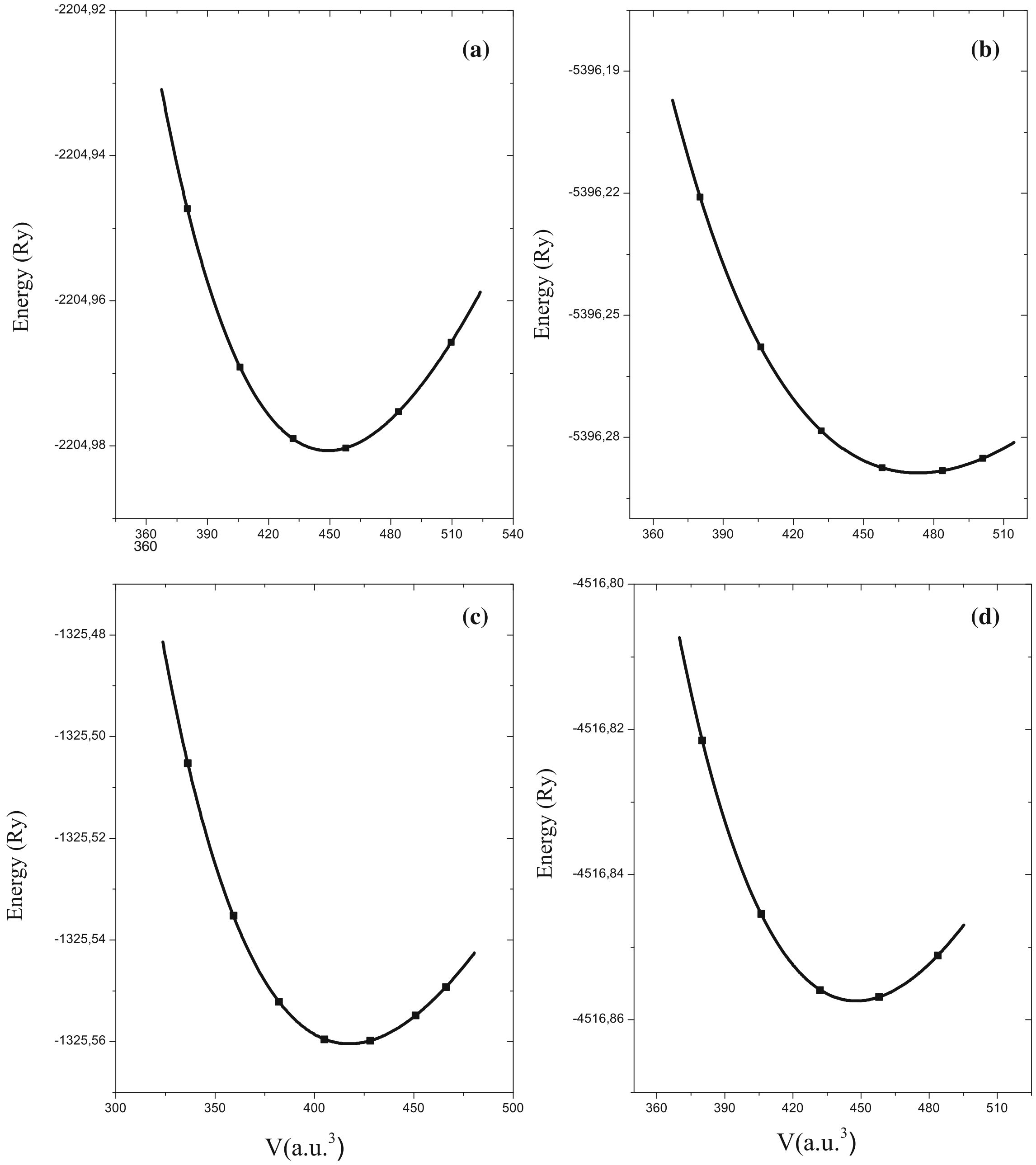

Fig. 1 Calculated total energy as a function of volume, (**a**) $KMgF_3$, (**b**) $KZnF_3$, (**c**) $NaMgF_3$ and (**d**) $NaZnF_3$

Table 1 Lattice constant a(Å), bulk modulus *B* (in GPa) pressure derivative of bulk modulus B' and energy gap *Eg* for ABF_3(A = K, Na; B = Mg, Zn) compounds

	Present work (FP-LAPW)	Present work (PW-PP)	Experiment	Other
$KMgF_3$				
a	4.052	4.133	3.978 ± 0.05 [28] 3.9897 [30], 3.9839 [36] 3.973 [52], 4.0060 [54] 3.993 [55]	3.91 [53] 4.0809 [54] 4.040 [59]
B''	67.53	81.564	71.2 [54],70.4 [56] 75.1 [57], 75.6 [58]	90.97 [53] 72.01 [54] 72.15 [59]
B’	4.422	–	4.7 [54]	4.64 [53] 4.65 [54] 4.68 [59]
Eg	7.37	7.56	12.4 [25]	7.03 [59]
$NaMgF_3$				
a	3.955	4.109	3.955 [32], 3.833 [60] 3.876 [61], 3.964 [70]	3.836 [62] 3.840 [63] 3.872 [64]
B	69.87	159.423	66. 8676 [70]	87.999 [62] 78.2 [64]
B'	4.146	–	–	3.97 [64]
Eg	6.40	6.39	–	5.90 [64] 5.99 [70][a] 6.74 [70][b] 10.6 [70][c]
$KZnF_3$				
a	4.124	4.241	4.05 [65], 4.056 [66] 4.0611 [67]	–
B	71.463	38.391	–	–
B’	4.50	–	–	–
Eg	4.06	4.43	–	–
$NaZnF_3$				
a	4.049	4.182	4.065 [70]	–
B	74.179	157.834	71.4526 [70]	–
B’	4.7566	–	–	–
Eg	3.38	4.09	–	3.35 [70] [a] 4.11 [70] [b] 6.60 [70] [c]

Experiment ([25], [28], [30], [36], [52], [54–61], [65–67])

Ref [53] using FP-LAPW-LDA

Ref [54] using FP-LMTO-GGA + LDA

Ref [59] using PAW-GGA

Ref [62] ab initio perturbed ion (*ai* PI)

Ref [63] using a priori calculation

Ref [64] using PP-PW-LDA

Ref [70][a] using FP-LAPW –GGA

Ref [70][b] using FP-LAPW –EV-GGA

Ref [70][c] using FP-LAPW–mBJ

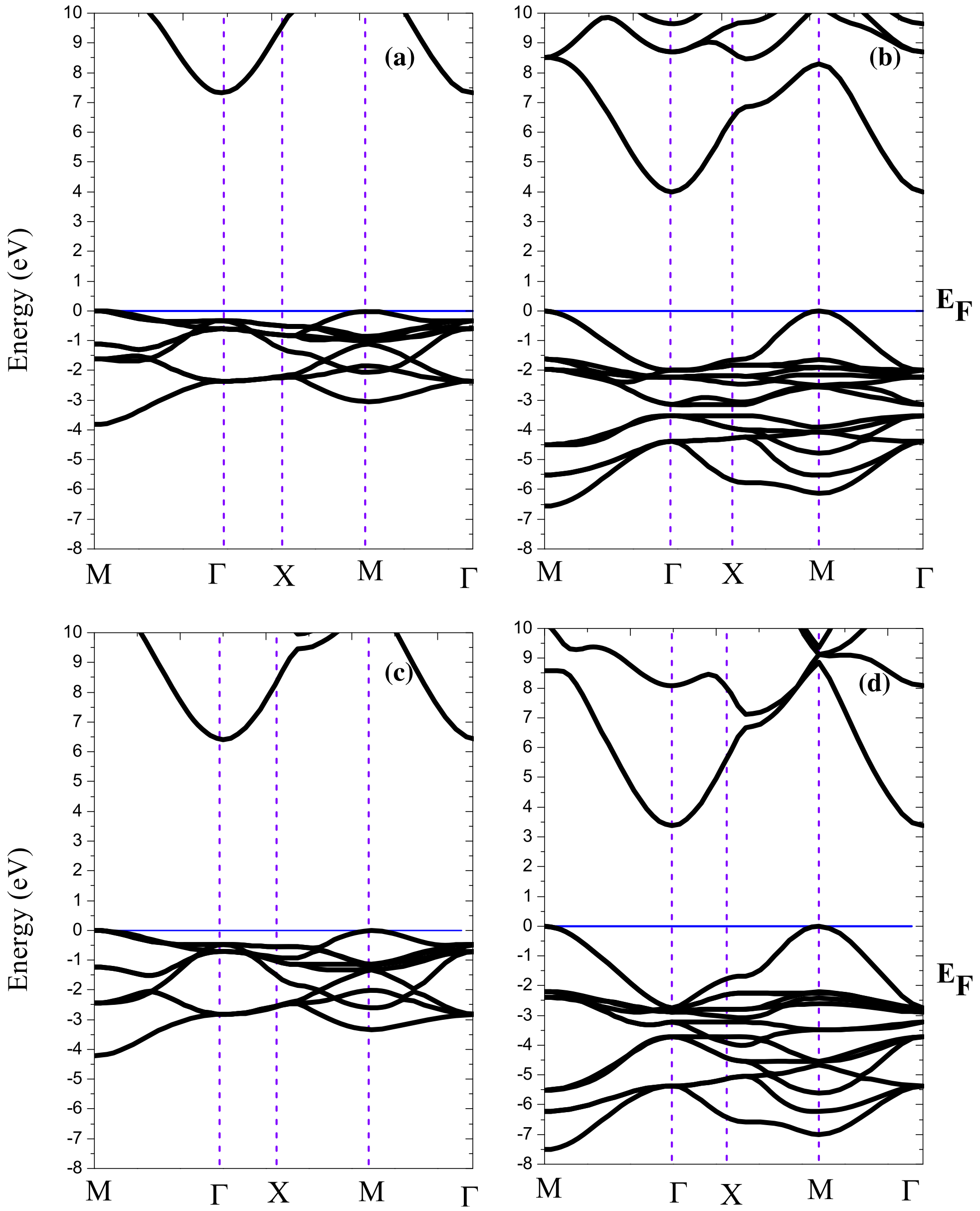

Fig. 2 Band structure for high-symmetry directions in the Brillouin zone, (**a**) $KMgF_3$, (**b**) $KZnF_3$, (**c**) $NaMgF_3$ and (**d**) $NaZnF_3$

plane wave (NCP) method within the density functional theory (DFT) with the generalized gradient approximation (GGA). The paper is organized as follows. The theoretical background is presented in Sect. 2. Results and discussion are presented in Sect. 3. A summary of the results is given in Sect. 4.

2. Computational method

Full-relativistic calculations of the electronic structure of ABF_3($A = K$, Na; $B = Mg$, Zn) are performed within the density functional theory [43] using Ab initio full-potential linearized augmented plane wave method [44] as implemented in WIEN2 K code Blaha et al. [45]. The Kohn–Sham equations are solved self-consistently using FP-LAPW method. In the calculations reported here, we use a parameter $R_{MT}K_{max} = 9$, which determines matrix size (convergence), where K_{max} is the plane wave cut-off and R_{MT} is the smallest of all atomic sphere radii. The radii R_{MT} of the muffin tins (MT) are chosen to be approximately proportional to the corresponding ionic radii. Exchange–correlation effects are treated using GGA as parameterized by Perdew et al. [46]. Self-consistent calculations are considered to be converged when the total energy of the system is stable within 10^{-4} *Ry*. The convergence criteria for total energy and force are taken as 10^{-5} and 10^{-4} eV/Å, respectively. The valence wave functions inside the spheres are expanded up to $l_{max} = 10$ while the charge density was Fourier expanded up to $G_{max} = 14$. The Monkorst-Pack

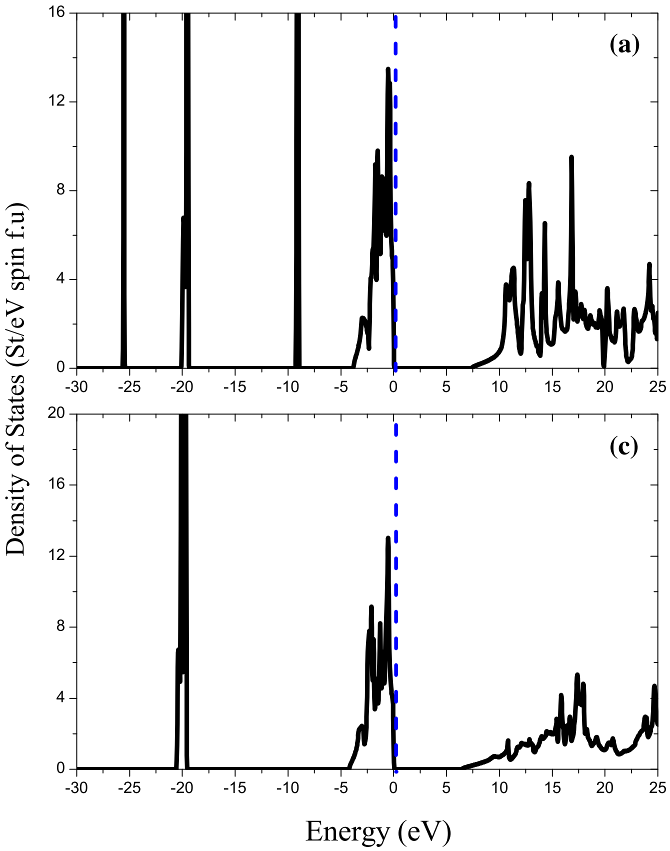

Fig. 3 Total density of states of (**a**) $KMgF_3$, (**b**) $KZnF_3$, (**c**) $NaMgF_3$ and (**d**) $NaZnF_3$

special k-points were performed using 3000 special k-points in the Brillouin zone. Calculations of the frequency-dependence of the optical properties were carried out using 8000 k-points in the Brillouin zone for the ABF_3 (A = K, Na; B = Mg, Zn) compounds.

Optical properties of a solid are usually described in terms of the complex dielectric function $\varepsilon(w) = \varepsilon_1(w) + i\varepsilon_2(w)$ The imaginary part $\varepsilon_2(w)$ was calculated from the momentum matrix elements between the occupied and unoccupied wave functions within the selection rules. The real part $\varepsilon_1(w)$ of the dielectric function was calculated by the Kramers–Kronig transformation [47] of the imaginary part $\varepsilon_2(w)$ Other optical constants were computed from the values of $\varepsilon_1(w)$

The norm-conserving pseudopotential (NCP) method [48] and the GGA approach according to Perdew-Burke-Ernzerhof [46] has been untilized in the present study. A computer program CASTEP (Cambridge Serial Total Energy Package) [49], was used tocalculate structural, electronic and optical properties of ABF_3 (A = K, Na; B = Mg, Zn) compounds. Besides, the kinetic cut-off energy for the plane wave expansion is considered to be 800 eV for all analyzed cases. The special points sampling integration over the Brillouin zone was employed by using the Monkhorst–Pack method with 20 × 20 × 20 k-points. Based on the Broyden Fletcher Goldfarb Shenno (BFGS) [50] minimization technique, the system reached the ground state via self-consistent calculation when the total energy is stable to within 5×10^{-6} eV/atom, and less than 10^{-2} eV/Å for the force.

3. Results and discussion

3.1. Structural properties

The main objective in this work is to calculate the total energy as a function of the unit-cell volume around the equilibrium cell volume V_0in ABF_3(A = K, Na; B = Mg, Zn) compounds, using FP-LAPW and PP-PW methods. Figure 1 presents the structural optimization curves obtained by using the FP-LAPW method; the results indicate that $KZnF_3$ compound is found to be energetically more favorable than $KMgF_3$, $NaMgF_3$ and $NaZnF_3$ compounds. Table 1 presents the calculated equilibrium lattice constants for the ABF_3(A = K, Na; B = Mg, Zn) compounds that are determined by fitting the total energy as a function of volume to the Murnaghan equation of state [51]. Moreover, in Table 1, our calculated values of a_0, B, and B' are compared with previous experimental and theoretical results. Based on

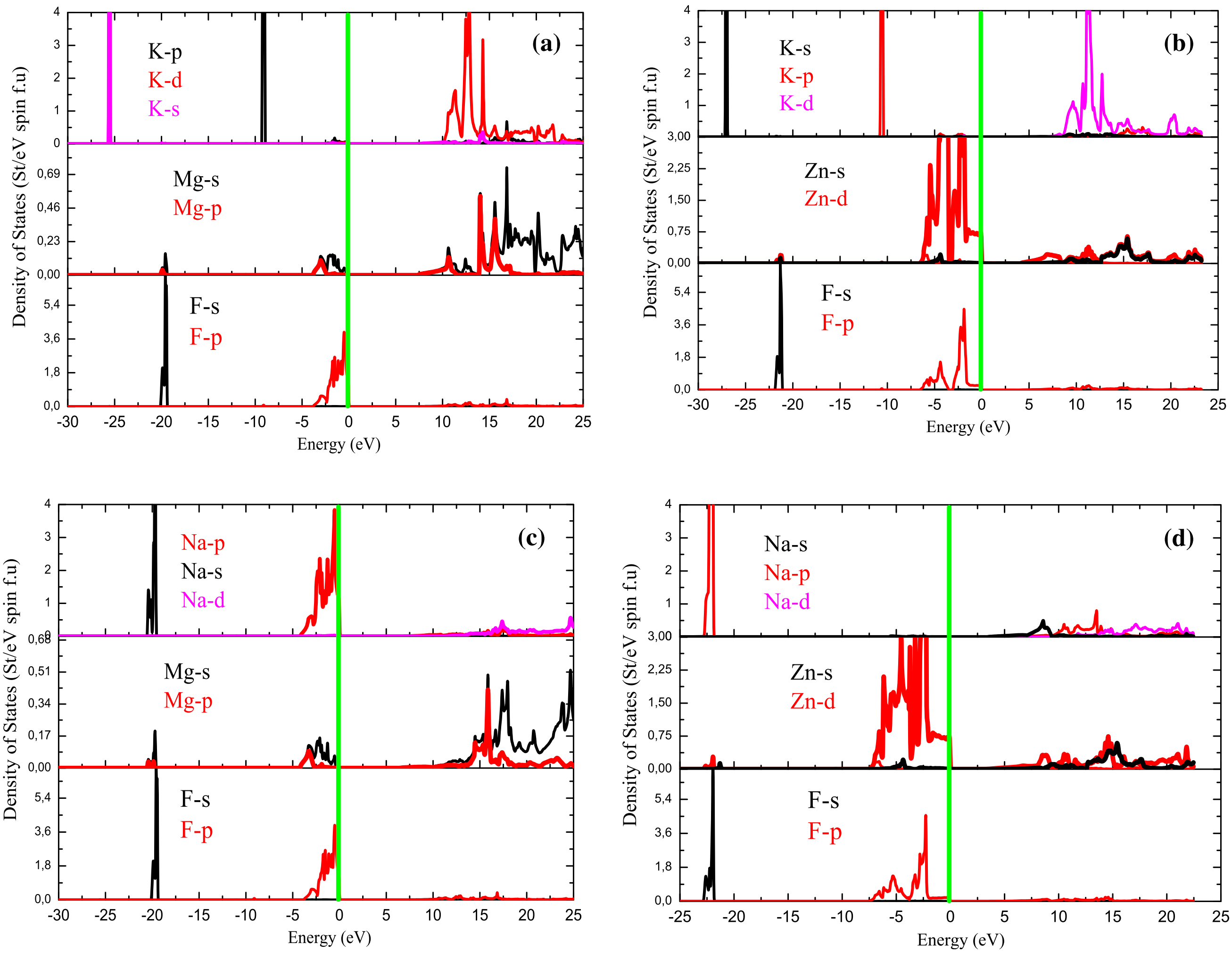

Fig. 4 Projected density of states of (**a**) $KMgF_3$, (**b**) $KZnF_3$, (**c**) $NaMgF_3$ and (**d**) $NaZnF_3$

the experimental data, the equilibrium lattice constants for $KMgF_3$, $KZnF_3$ and $NaMgF_3$ are best described by FP-LAPW, compared with the PW-PP method. Nevertheless, both used methods overestimated the lattice constant with respect to experiment. This is not surprising; the results are consistent with the general trend of the GGA approach [68, 69]. For the $KMgF_3$compound, the calculated bulk modulus by FP-LAPW is in better agreement with the experiment compared to that obtained by PP-PW. Knowing that the structural stability, mechanical, electronic and thermodynamic properties of $NaXF_3$ (X = Mg, Zn) compounds that was predicted by Arar et al. [70].

3.2. Electronic properties

The band structures of ABF_3 (A = K, Na; B = Mg, Zn) have been calculated at the theoretical equilibrium lattice constant using both FP-LAPW and PP-PW methods. Because of the similarity in the most estimated results, only FP-LAPW results are presented. The energy band structure calculated along the high symmetry directions in the Brillouin zone, is illustrated in Fig. 2. The valence band maximum (VBM) is located at the *M* point, whereas the conduction band minimum (CBM) is located at the *Γ* point. The energy gap values obtained from the FP-LAPW approach are 7.37, 6.40, 4.06 and 3.38 eV, while those obtained from the PP-PW calculations are 7.56, 6.39, 4.43 and 4.09 eV, for $KMgF_3$, $NaMgF_3$, $KZnF_3$ and $NaZnF_3$, respectively.This band structure is representative of wide gap fluoroperovskite with indirect gaps insulator. For KMgF3, the calculated indirect band gap for both methods, which is much smaller than the measured experimental value of 12.4 eV [25] (a well-known deficiency of DFT approach), however, in good agreement with the previously reported calculated values at 7.24 eV [53] and 7.03 eV [59].

In the next stage, we presented the partial densities of states of these compounds as illustrated in Figs. 3 and 4. The Fermi level was set as 0 eV. Basically, for $KMgF_3$ and $KZnF_3$ compounds, the DOS can be divided into three parts, at lower energy where we find the contribution of K-s and

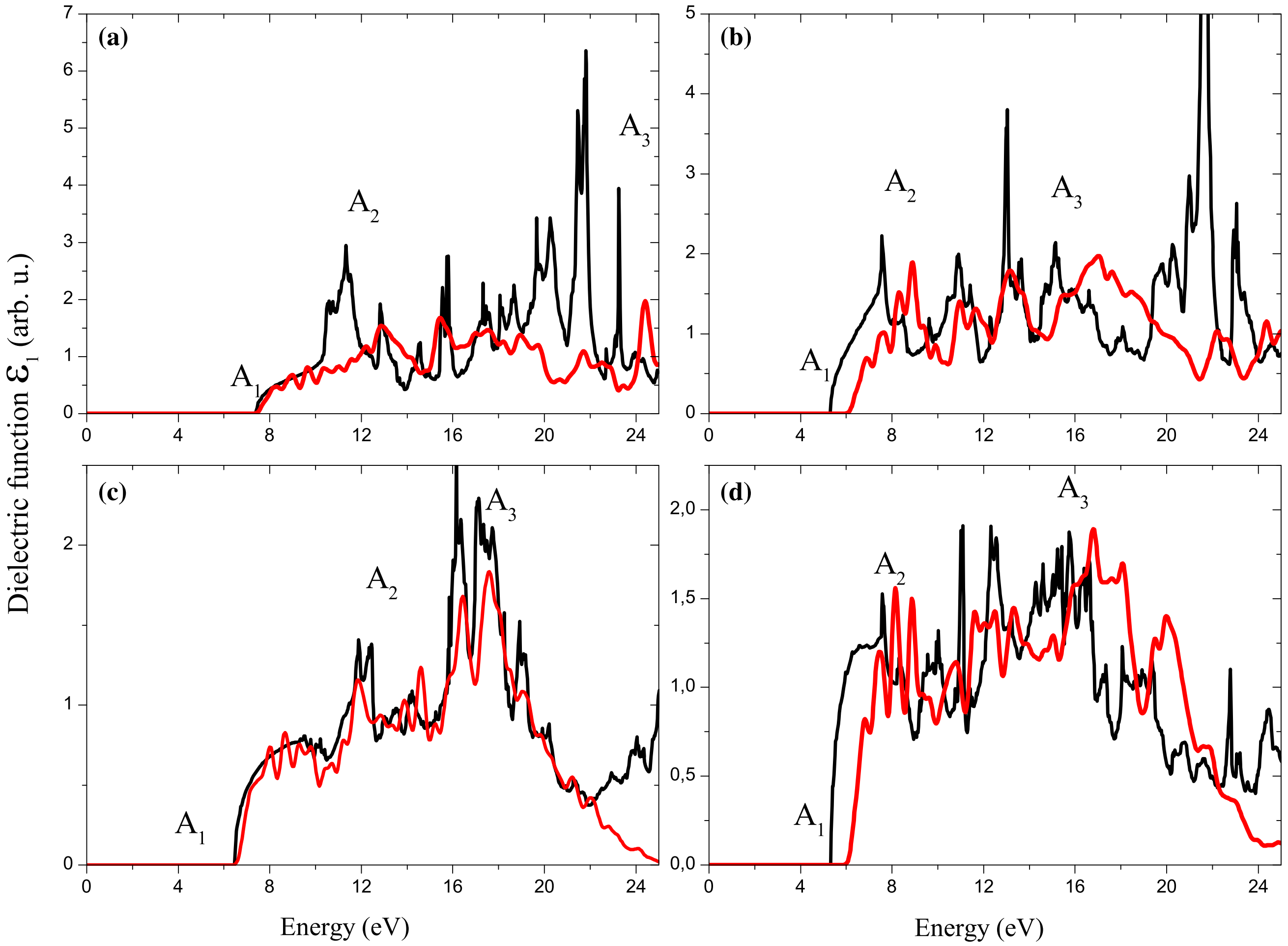

Fig. 5 The calculated real part of dielectric function for (**a**) $KMgF_3$, (**b**) $KZnF_3$, (**c**) $NaMgF_3$ and (**d**) $NaZnF_3$

F-s states; the second part is from −15 to 0 eV that is mainly derived from K-p and F-p states for $KMgF_3$ compound, and K-s, Zn-d and F-p electrons for $KZnF_3$ compound, the third part which is beyond the Fermi level, where the contribution is due to K-d and Zn–s states for $KZnF_3$ compound, where the K-d, s and p orbitals of Mg atoms create fully unoccupied bands for $KMgF_3$ compound. Furthermore, for the $NaMgF_3$ and $NaZnF_3$, a few F-s and Na-s states observed to occur at lower energies. The contribution of Zn-d and F-p states for $NaZnF_3$appears from −15 eV to 0 eV and the conduction band is mainly derived from Na-d and Zn–s states. It has been seen for the $NaMgF_3$ compound, from −15.0 to 0 eV, which represents the contribution of the p orbitals of Na atoms hybridized with F-p states and the conduction band, is mainly derived from Na d states hybridized with s and p electrons for Mg atoms.

3.3. Optical properties

Mainly, the dielectric function, refractive index and extinction coefficients at the equilibrium lattice constant were calculatedusing both FP-LAPW and PP-PW approaches.

In Fig. 5 and 6 we present the dielectric function of ABF_3(A = K, Na; B = Mg, Zn) compounds that calculated by FP-LAPW(black line) and PP-PW (red line) methods, respectively.For energies up to 25 eV, based on our calculated band structure it would be worthwhile to identify the interband transitions that are responsible for the structure in $\varepsilon_2(\omega)$ Our analysis of the $\varepsilon_2(\omega)$ spectra shows that the threshold energy (first critical point) of the dielectric function occurs at about A_1 (Table 2) for$KMgF_3$ and $NaMgF_3$compounds. These points are mainly initiated from the electron transition from the F-p (VB) and Na- p (VB) to Mg- p (CB) orbitals. One can note that in $KMgF_3$ and $NaMgF_3$ compounds, the ε_2 *(ω)* spectrum shows a peaks A_2 and A_3 (Fig. 5), respectively. These peaks are mainly derived from the transition from K-p (VB) to Mg- p(CB) and F-s (VB) and Na-s (VB) to Mg-s (CB) orbitals, respectively. In the case of $KZnF_3$ and $NaZnF_3$ compounds, the peaks are A_1, A_2 and A_3 (Fig. 5) which are mainly derived from the transition

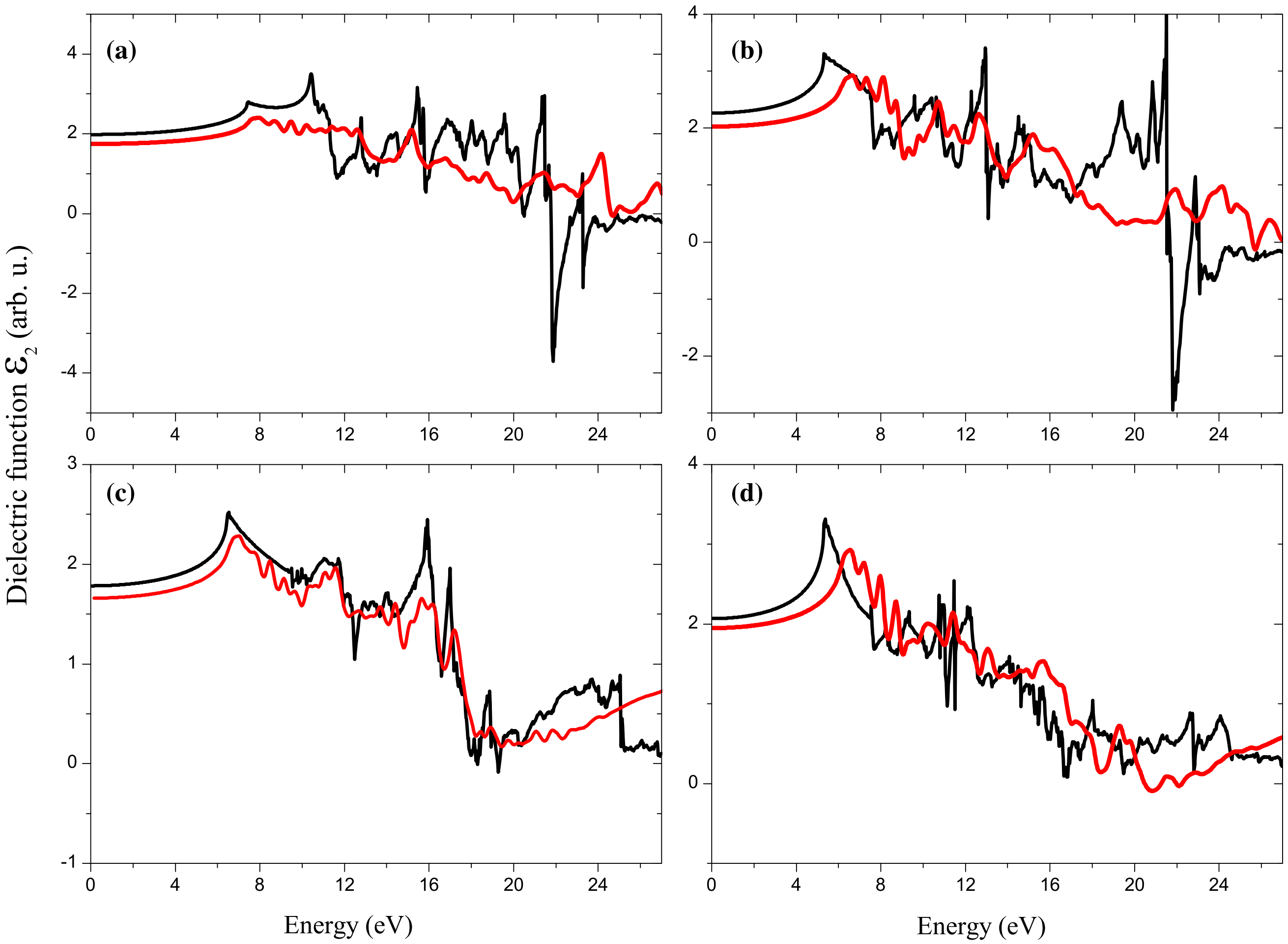

Fig. 6 The calculated imaginary part of dielectric function for (**a**) $KMgF_3$, (**b**) $KZnF_3$, (**c**) $NaMgF_3$ and (**d**) $NaZnF_3$

Table 2 Position of the principal peaks of the imaginary part of the dielectric function for ABF_3(A = K, Na; B = Mg, Zn) compounds

	A1	A2	A3
$KMgF_3$			
FP-LAPW	7.15	11.32	21.71
PW-PP	7.18	12.87	24.33
$NaMgF_3$			
FP-LAPW	6.17	12.29	17.24
PW-PP	6.27	12.00	17.63
$KZnF_3$			
FP-LAPW	5.24	7.55	15.03
PW-PP	6.01	8.82	16.88
$NaZnF_3$			
FP-LAPW	5.13	7.56	15.63
PW-PP	6.11	8.15	16.98

Table 3 Calculated, experimental and theoretical values of static constants ε_0, refractive index n_0

	Methods	Present work ε_0	Experiment ε_0	Other ε_0	Present work $n(0)$
$KMgF_3$	FP-LAPW	1.98	2.04 [70]	2.14 [59]	1.40
	PW-PP	1.74	–	–	1.30
$NaMgF_3$	FP-LAPW	1.78	–	–	1.32
	PW-PP	1.65	–	–	1.28
$KZnF_3$	FP-LAPW	2.26	–	–	1.44
	PW-PP	2.02	–	–	1.42
$NaZnF_3$	FP-LAPW	2.07	–	–	1.50
	PW-PP	1.95	–	–	1.39

from Zn-d (VB) and F-p(VB) to K-d (CB), K-s(VB) to K-d(CB) and F-s(VB)and Na-d (VB) to K-d(CB) orbitals, respectively. The behaviour of $\varepsilon_1(\omega)$ seems to be rather similar to that of $\varepsilon_2(\omega)$ below the reststrahlen region in the optical spectra, the real part of the dielectric function asymptotically approaches the static or low-frequency dielectric constant ε_0. The calculated dielectric constant ε_0 and the static refractive index n_0 of these compounds using FP-LAPW and PP-PW methods are reported in Table 3. The present investigation shows that the dielectric constant ε_0 of the studied compounds varies from 1.74 to 2.26. Our results for the dielectric constant ε_0 of $KMgF_3$ compound for both methods are in good agreement with previous theoretical and experimental data [59, 71].

The refractive index and the extinction coefficient are displayed in Figs. 7 for FP-LAPW and PP-PW methods, respectively. Note that the calculated data show clear peaks originating from the excitonic transitions at the E_0 edges. The strongest peaks in $n(\omega)$ spectra are related mainly to the 2D exciton transition (E_1) [72]. In this context, using FP-LAPW method, the static refractive index n_0 is found to be 1.40, 1.32, 1.44 and 1.50 for $KMgF_3$, $NaMgF_3$, $KZnF_3$ and $NaZnF_3$ compounds. These values differ largely from those of 1.30, 1.28, 1.42 and 1.39 obtained using PP-PW method, respectively. As a matter of fact, in the absence of both experimental and theoretical data of the refractive index and extinction coefficients for the material of interest, so to the best of our knowledge, no comment can be

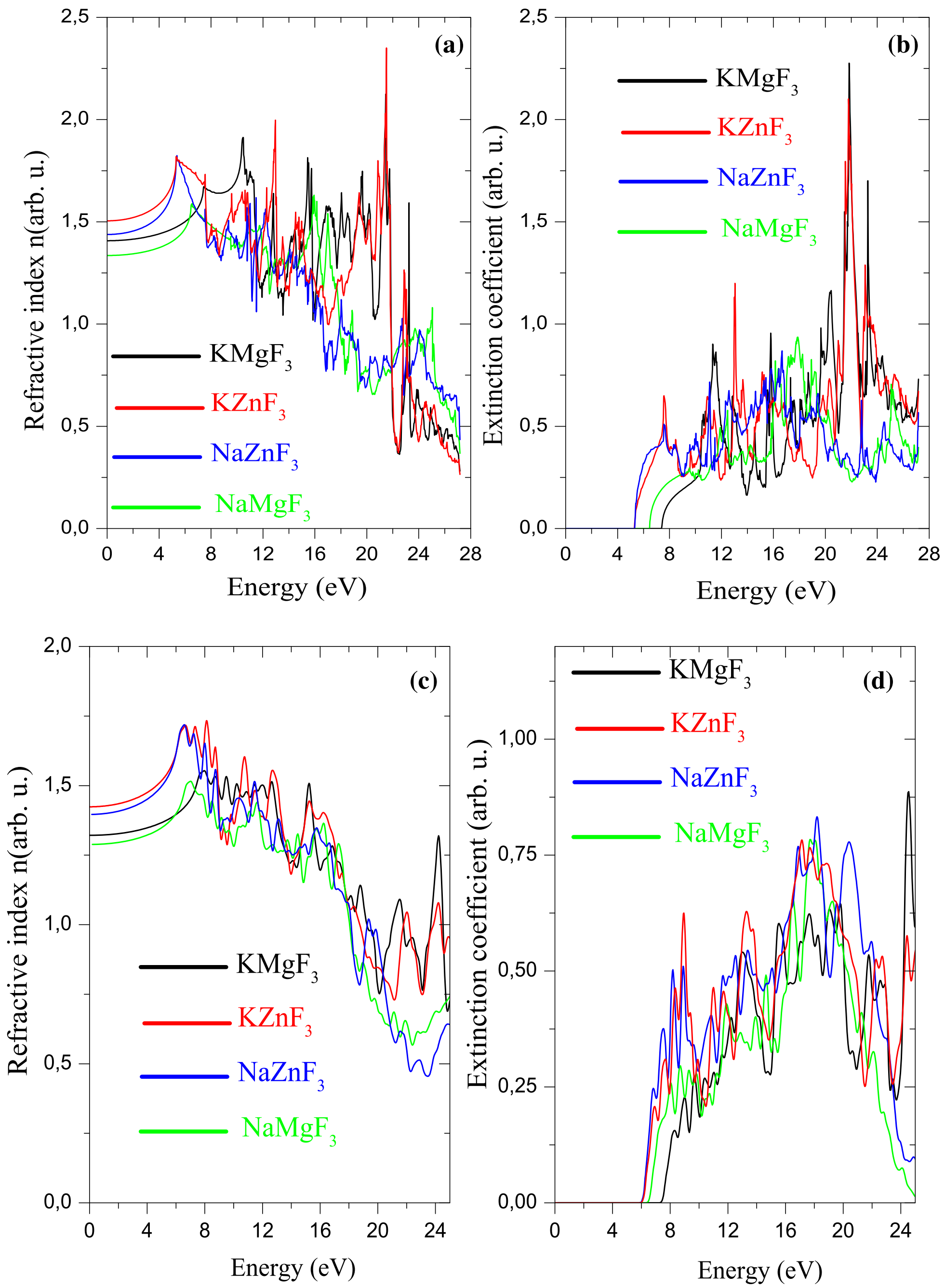

Fig. 7 Calculated (**a**) refractive index *n*(*w*) using FP-LAPW, (**b**) refractive index *n*(*w*) using PP-PW, (**c**) extinction coefficient using FP-LAPW, (**b**) extinction coefficient using PP-PW method

ascribed to the accuracy of the two used methods and hence our results may serve only for a reference.

4. Conclusions

In summary, we have calculated the structural, electronic and optical properties of fluoroperovskites ABF3(A = K, Na; B = Mg, Zn) using first principle. The ground state properties of these compounds such as equilibrium lattice constant, bulk modulus demonstrated a good agreement with the experimental results. The first principles calculations were adopted to study the electronic structures of ABF_3 (A = K, Na; B = Mg, Zn) compounds and the results indicated that these four compounds are indirect band gap insulator. The optical properties are analysed and the origin of some peaks in the spectra is discussed. Besides, the dielectric function ε (ω), refractive index n (ω), and extinction coefficient K (ω) for radiation up to 25 eV have also been reported and discussed.

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