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Comparative First-Principles Study of Structural Stability, Mechanical Behavior, Electronic Structure, and Optical Response of $CaCl_2$ and CaF_2

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Abstract
This study presents a comprehensive first-principles investigation of the structural, elastic, electronic, and optical properties of cubic $CaCl_2$ and CaF_2 compounds using density functional theory (DFT). The calculations were performed within the full-potential linearized augmented plane wave (FP-LAPW) framework. Structural optimization confirms that both compounds crystallize in a stable cubic phase, with equilibrium lattice parameters in good agreement with expected values. Elastic constant calculations satisfy the Born stability criteria, indicating mechanical stability of both materials, while comparative analysis reveals that CaF_2 exhibits higher stiffness, bulk modulus, and ductility than $CaCl_2$. Electronic band structure and density of states analyses demonstrate that both compounds are wide band gap insulators with indirect band gaps, where CaF_2 shows a larger band gap due to stronger ionic bonding and higher electronegativity of fluorine. Optical properties, including dielectric function, absorption coefficient, reflectivity, and energy loss function, indicate negligible activity in the visible region and strong response in the ultraviolet range. CaF_2 exhibits sharper and more intense optical peaks, suggesting superior performance in high-energy optical applications. Overall, the results highlight the potential of these materials, particularly CaF_2 for use in ultraviolet optoelectronic devices and dielectric applications.

Keywords: Density functional theory (DFT); FP-LAPW method; WIEN2k; Elastic properties; Electronic structure; Optical properties

Introduction
The alkaline earth metal halides have been of interest in condensed matter physics and materials science as they have simple crystal structures, strong ionic bonding, and a large band-gap insulating character. Of these compounds, calcium-based halides, including $CaCl_2$ and CaF_2 have been the focus of significant interest due to their impressive structural stability and promising optical characteristics. CaF_2, which forms in the fluorite structure, is commonly known to be very transparent in a large spectrum of the light especially in the ultraviolet (UV) region, and is thus a very essential material in optical lens and windows and laser systems. Conversely, $CaCl_2$, which has not received such intensive attention as optical applications, offers a valuable parallel system to study the effects of halogen substitution on electronic and optical behavior [1-4].
The fast growth of computational materials science has made it possible to investigate the properties of materials in detail with first-principles methods. Specifically, the density functional theory (DFT), which was originally developed by Pierre Hohenberg and Walter Kohn, has become one of the keystone methods to accurately predict structural, electronic, and optical properties [5,6]. A number

of studies have, using DFT-based methods, verified that alkaline earth halides have wide band gaps and ionic character with their valence bands being dominated by the halogen p-orbitals and the conduction bands by the metal s- and d-states [79]. The electronegativity of fluorine and chlorine are also important in the determination of the electronic structure, which makes the electronic states more localized, and the band gap in CaF_2 larger than in $CaCl_2$.

The optical properties like the dielectric function, absorption coefficient, reflectivity, refractive index, and energy loss function are essential in the study of the electromagnetic radiation interaction with matter. These properties are directly connected with the electronic structure and give useful insights of interband transitions and polarization effects. Wide band gap materials, including CaF_2 and $CaCl_2$ are especially useful in applications in UV optics, photonic devices, and high-frequency dielectric components because of their low absorption in the visible and strong performance at higher photon energies [10-12]. Experimental and theoretical studies have shown that CaF_2 has better optical characteristics, such as high transparency, low refractive index, and high radiation resistance and is favored in the fabrication of advanced optical systems [13-15]. In the meantime, $CaCl_2$ indicates relatively wider optical characteristics and increased polarizability in lower photon energies which can be beneficial in certain dielectric applications [16].

Along with optical properties, structural, elastic, and electronic properties of these materials are required to analyze their overall performance in real-life applications. It has been previously noted that CaF_2 has more mechanical strength and stiffness than $CaCl_2$ due to its stronger ionic bonding and smaller crystal structure [17, 18]. Moreover, the connection between the electronic structure and optical response indicates that the thorough theoretical studies are essential to predict the material behavior in the most precise way.

Here, this research paper seeks to give a systematic first principle exploration of the structural, elastic, electronic and optical characteristics of $CaCl_2$ and CaF_2 in the cubic form. Through a comparative study, this paper aims to explain the mechanisms behind their characteristics in terms of physical principles, as well as evaluate their possible uses in optoelectronic and ultraviolet optical devices.

Computational Methodology

The structural, elastic, electronic, and optical properties of the studied compounds CaX (X = Cl, F) were calculated with the full-potential linearized augmented plane wave method, which is a part of the density functional theory, and which is done with the WIEN2k software [19]. The Tran-Blaha-modified Becke-Johnson potential (TB-mBJ) functional was used because it is known to be better in the description of the electronic and optical characteristics of materials [20].In the calculation of structural optimization and elastic property, the exchange-correlation potential was calculated using the Generalized Gradient Approximation because it gives accurate values of ground-state properties [21]. The FP-LAPW basis set was determined by the following parameter: RMT*Kmax, with suitable muffin-tin radii (RMT) chosen to provide convergence. An energy separation of 6.0 Ry was used to distinguish between core and valence states. The self-consistent field (SCF) calculations were regarded to be converged when the change in the total energy between consecutive calculations was lower than 0.001 Ry. The equilibrium structural parameters were obtained by fitting the total energy versus volume data using the Birch–Murnaghan equation of state [22].The IRelast package [23], was used to determine the elastic constants, which allowed to evaluate mechanical stability and other related elastic properties. In addition, the optical characteristics were studied by applying the complex dielectric function which gives the information of the interaction of electromagnetic radiation with the material [24].

Results and Discussion

Structural Properties

The density functional theory of cubic crystal system was used to analyze the structural properties of the investigated compounds. Both compounds are in the space group Fm-3m space group (No. 225) and crystallize in the face-centered cubic structure. In the case of the $CaCl_2$ structure, the optimum lattice parameters were determined to be a=b=c=6.71 Å which corresponds to a very symmetrical cubic structure. These atomic positions can be identified as a $CaCl_2$ type, with Ca atoms at the origin

(0, 0, 0), and Cl atoms at fractional positions (0.25, 0.75, 0.75). Likewise, CaF_2 compound also takes the cube symmetry with lattice constants a=b=c=5.52 Å. Ca atoms are situated at (0, 0, 0) and F atoms at the (0.25, 0.75, 0.25) positions which is also in accordance with fluorite type structure. As an improvement in gaining more accurate equilibrium structural parameters, we fitted the total energy as a function of volume with the Birch-Murnaghan equation of state. This fitting results in optimized lattice constants of a_0=6.7538 Å $CaCl_2$ and a_0=5.5288 Å CaF_2 which are in good agreement with the starting structure inputs and indicates that the cubic phase is stable.

The ground state energies were determined to be -3207.314172Ry of $CaCl_2$ and -1760.899414Ry of CaF_2, the stable structures of which are found at the equilibrium volume. The balance volumes are 519.7285a.u^3 and 285.1170a.u^3 respectively. Moreover, the mechanical properties were considered by the bulk modulus (B) and its pressure derivative B. The values of the bulk modulus were determined to be 40.0178 GPa $CaCl_2$ and 78.6716 GPa CaF_2, indicating that CaF_2 is relatively less compressible and more mechanical in nature than $CaCl_2$. The pressure derivatives of bulk modulus were determined to be B′=4.0609 and B′= 5.1367 respectively, which is a normal compressibility behavior with applied pressure.

In general, the structural analysis shows that both compounds are stable in cubic phase, but the structural rigidity of CaF_2 is greater than that of $CaCl_2$ because of the higher bulk modulus.

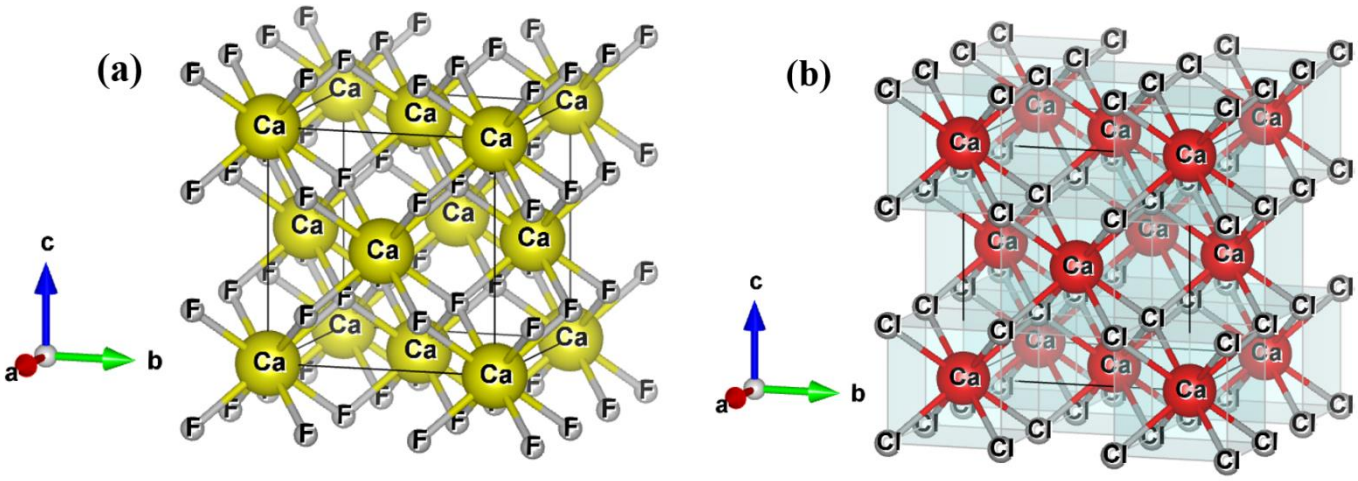

Fig. 1: Schematic representation of the optimized cubic structures of (a) $CaCl_2$ and (b) CaF_2

Table 1: Presents the calculated structural parameters, including the lattice constant a_0, bulk modulus B, its pressure derivative B′, equilibrium volume V_0, and ground state energy E_0 for $CaCl_2$ and CaF_2 compounds

Parameters	$CaCl_2$	CaF_2
1. a_o (Å)	6.7538	5.5288
2. E_o (Ry)	-3207.314172	-1760.899414
3. V_o (a.u^3)	519.7285	285.1170
4. B (GPa)	40.0178	78.6716
5. B'	4.0609	5.1367

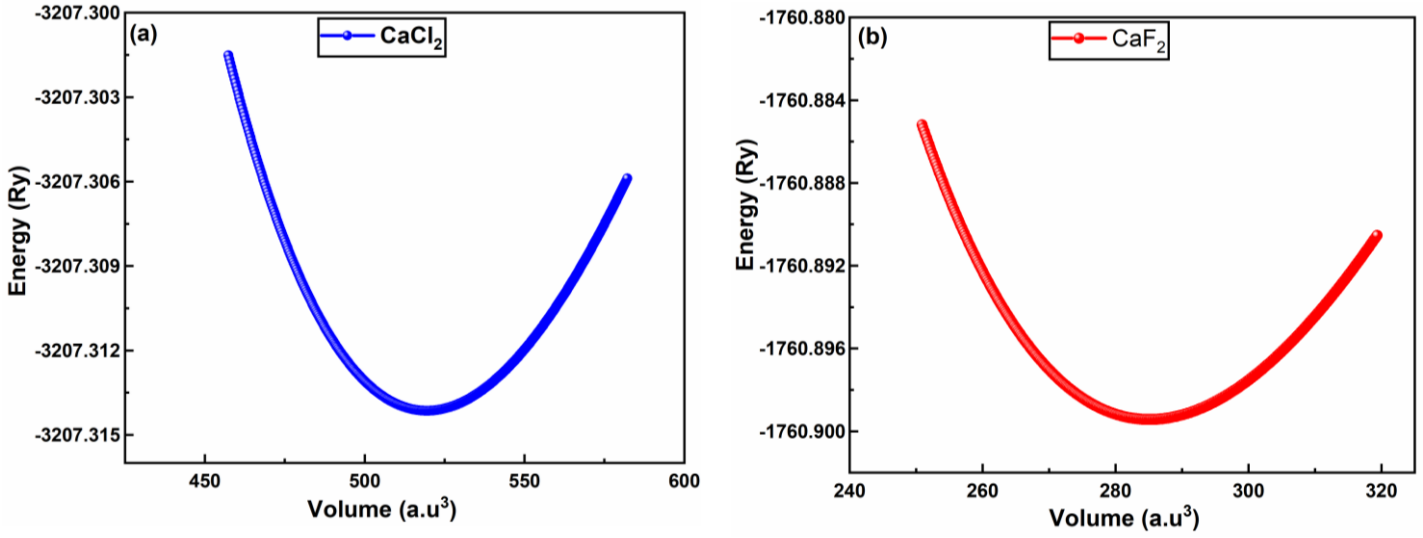

Fig. 2: Variation of total energy as a function of unit-cell volume for (a) $CaCl_2$ and (b) CaF_2

Elastic Properties

Elastic Properties

The elastic properties of $CaCl_2$ and CaF_2 were investigated to evaluate their mechanical stability and response to external stress. For cubic crystals, the independent elastic constants are C_{11}, C_{12} and C_{44} which fully describe the mechanical behavior of the system.The calculated elastic constants for $CaCl_2$ are C_{11}=109.84 GPa, C_{12}=4.92GPa, and C_{44}=24.74 GPa, while for CaF_2, the values are C_{11}=154.20 GPa, C_{12}=44.14 GPa, and C_{44}=34.94 GPa. These values satisfy the Born stability criteria ($C_{11}-C_{12}>0$, $C_{11}+2C_{12}>0$, $C_{44}>0$), confirming that both compounds are mechanically stable in the cubic phase.
The bulk modulus B, which is the ability to resist compression of volume is calculated as 39.89 GPa in $CaCl_2$ and 80.96GPa in CaF_2. CaF_2 has a greater bulk modulus which means that it is much less compressible and mechanically more rigid than $CaCl_2$. This pattern coincides with the analysis of the structure. The shear modulus G, the ability to resist deformation of the shape is determined to be 33.60Gpa for $CaCl_2$ and 41.94GPa for CaF_2. Likewise, the modulus Y, a measure of stiffness, of $CaCl_2$ and CaF_2 are 82.72GPa and 109.54GPa, respectively, confirming once again the increased stiffness of CaF_2. Pugh ratio (B/G) was used to determine the ductility and brittleness of the materials. The values determined are 1.19 of $CaCl_2$ and 1.93 of CaF_2. As materials with B/G less than 1.75 are brittle, $CaCl_2$ is brittle whereas CaF_2, with B / G greater than 1.75, is ductile. The ratio of the Poisson ν gives a clue on the type of interatomic bonding. The values obtained are 0.154 and 0.274 respectively. A relatively low value of $CaCl_2$ shows that there is a stronger directional (covalent-like) bond whereas the higher value of CaF_2 indicates a stronger ionic bond. The anisotropy factor A was used to measure elastic anisotropy. The values of A=0.472 of $CaCl_2$ and A=0.635 of CaF_2 are not unity and thus both of the compounds are anisotropic elastically, with CaF_2 being less anisotropic than $CaCl_2$.Also, Voigt shear modulus Gv values of $CaCl_2$ and CaF_2 are 35.83GPa and 42.98GPa respectively, which are in line with the general tendency of increased mechanical strength in CaF_2.To conclude, both compounds are mechanically stable but CaF_2 has shown better mechanical strength, better stiffness, and ductile properties over $CaCl_2$ compound, which is relatively softer and brittle.

Table 2: Calculated elastic parameters for $CaCl_2$ and CaF_2 compounds utilizing the IRelast module.

Elastic Parameters	$CaCl_2$	CaF_2
C_{11}	109.837609	154.196265
C_{12}	4.922004	44.13712
C_{44}	24.743095	34.938806
Y	82.720	109.543
G	33.601	41.944

A	0.472	0.635
v	0.154	0.274
B	39.889	80.96
B/G	1.187134619	1.930174345
G_v	35.829	42.975

Elastic Anisotropy (2D and 3D)

Directional dependence of elastic properties of CaF_2 and $CaCl_2$ is shown using 2D and 3D plots of Young's modulus, shear modulus and Poisson ratio. The non-circular shape of the 2D plots and the non-spherical shape of the 3D surfaces prove the anisotropy of the two compounds.CaF_2 is more symmetric and smooth on a relative scale, which means that there is less elastic anisotropy and more uniform mechanical behavior. $CaCl_2$ on the other hand exhibits more pronounced distortions in 2D and 3D plots, indicating that elastic properties are more directionally dependent. On the whole, the results indicate that both materials are anisotropic, although $CaCl_2$ is much more anisotropic than CaF_2, as the anisotropy factor calculated.

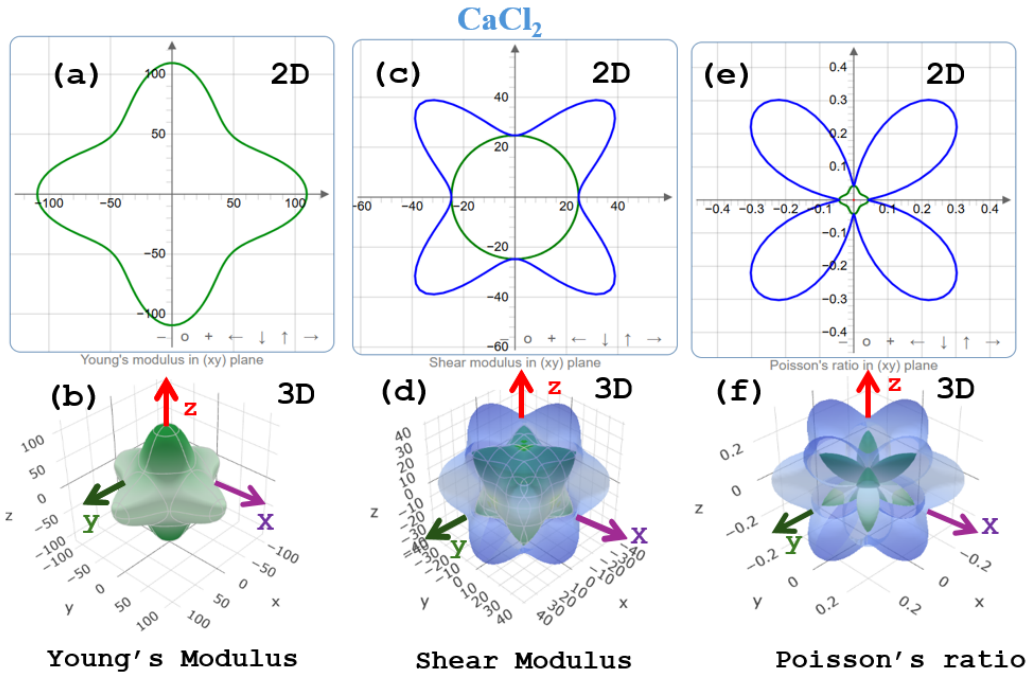

Fig 3: Elastic anisotropy in $CaCl_2$ shown via 2D contours and 3D surfaces of Young's modulus, shear modulus, and Poisson's ratio, highlighting direction dependent mechanical behavior.

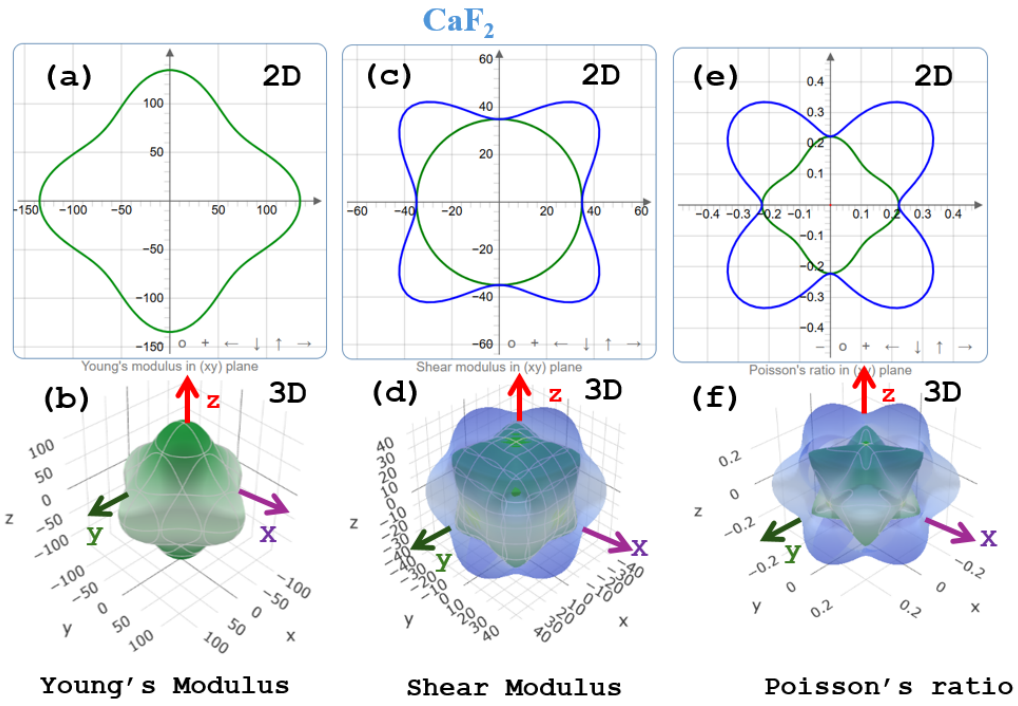

Fig 4: Elastic anisotropy in CaF_2 shown via 2D contours and 3D surfaces of Young's modulus, shear modulus, and Poisson's ratio, highlighting direction dependent mechanical behavior.

Comparison of Elastic Moduli

The bar chart shows the comparative analysis of the elastic moduli of $CaCl_2$ and CaF_2 and the dispersion of Young modulus (Y), shear modulus (G) and bulk modulus (B). As can be seen, CaF_2 shows much larger values of the three moduli in comparison with CaCl2.In particular, the modulus of the Young of $CaCl_2$ and CaF_2 are about 82.72 GPa and 109.54 GPa respectively, which is a sign of increased hardness of CaF_2. Equally, shear modulus increases to 41.94 GPa compared to 33.60 GPa indicating increased shear deformation resistance. The bulk modulus equally increases significantly by 39.89 GPa to 80.96 GPa, which proves that CaF_2 is much less compressible. On the whole, this comparison shows that CaF_2 has better mechanical strength and rigidity, and $CaCl_2$ has rather lower resistance to deformation and compression.

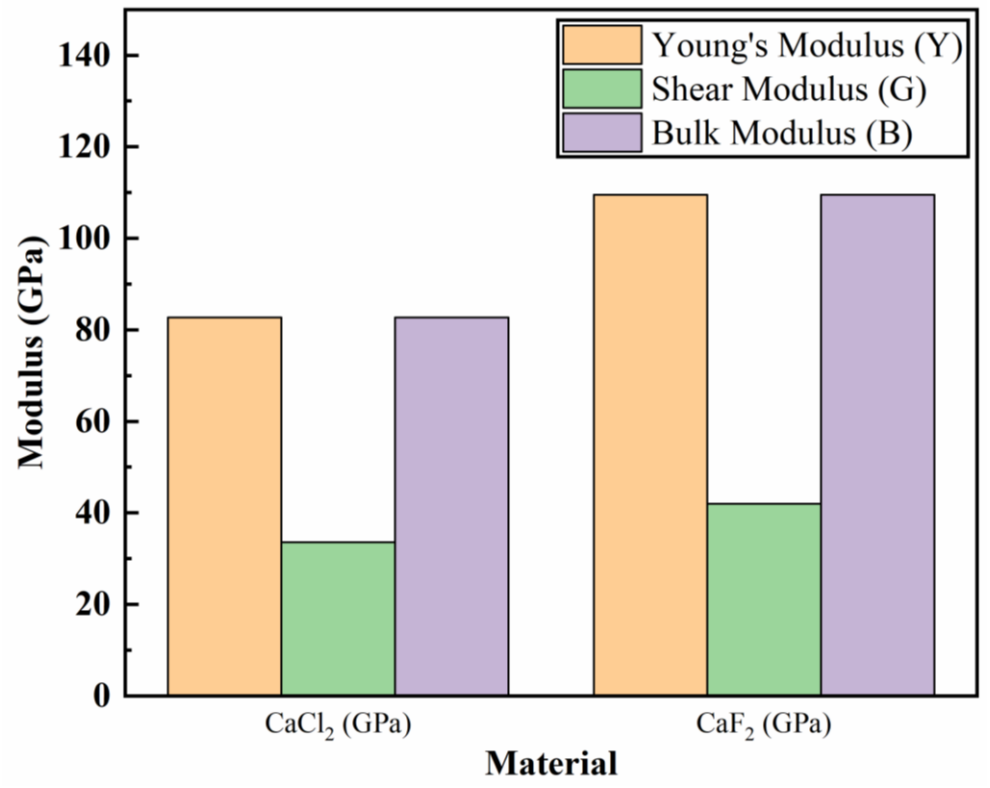

Figure 5: Elastic moduli of $CaCl_2$ and CaF_2: Young's modulus (Y), shear modulus (G) and bulk modulus (B), showing higher resistance to tensile and volumetric deformation than to shear.

Electronic Properties

The electronic properties of $CaCl_2$ and CaF_2 are studied based on the calculated band structures and density of states (DOS), and the results show apparent insulating properties of the two compounds. The fact that at the Fermi level (E_F = 0 eV) there are no electronic states indicates that neither material is a metal or a semiconductor, but rather falls into the category of wide band gap insulators. The valence band maximum (VBM) of $CaCl_2$ is below the Fermi level and the conduction band minimum (CBM) appears at higher energy at a different high-symmetry k-point, which is indicative of an indirect nature of the band gap. An analogous indirect transition is found in CaF_2 but the energy gap between the conduction and valence bands is much greater, indicating that CaF_2 has a broader band gap and greater insulating properties.

The complete and partial DOS give additional information on the orbital contributions. The valence band in either of the materials is dominated by the p-orbitals of the halogen atoms (Cl-p in $CaCl_2$ and F-p in CaF_2) with some minor mixing in with Ca states. Ca-derived states are primarily found in the conduction band, especially Ca-d orbitals, which suggests electronic excitation is a charge transfer between halogen p-states and Ca states. It is important to note that in CaF_2 the F-p states are more localized than the Cl-p states in $CaCl_2$ and this is one of the reasons that cause the band gap to widen. This is because of the increased electronegativity of fluorine which results in greater ionic bonding and less orbital overlap. In general, $CaCl_2$ and CaF_2 are indirect wide band gap insulators with CaF_2 having a relatively large band gap. Such electronic properties indicate that they can be used in applications in dielectric and optoelectronics devices, and especially in ultraviolet-transparent system where large band gap materials are needed.

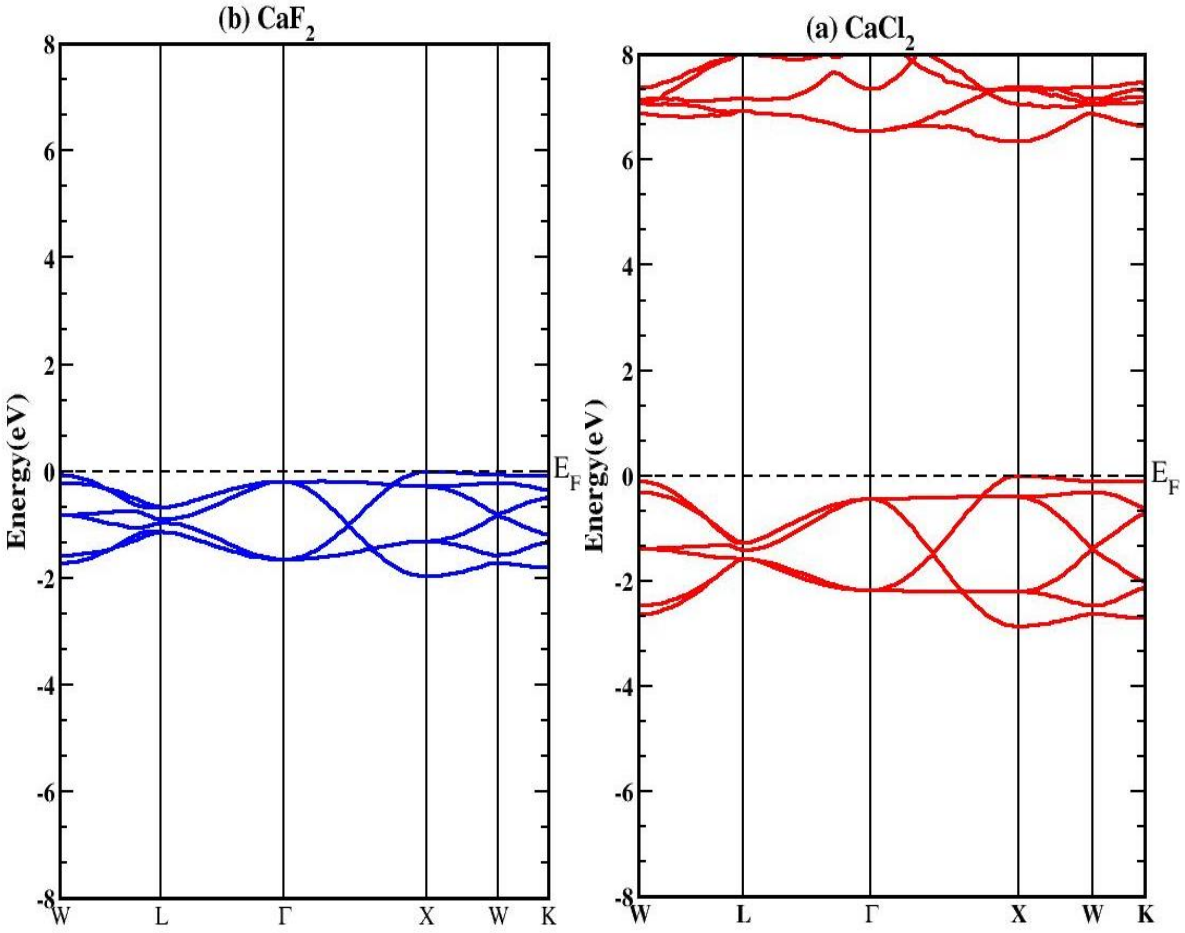

Fig 6: Band Structure and Density of States of $CaCl_2$ and CaF_2

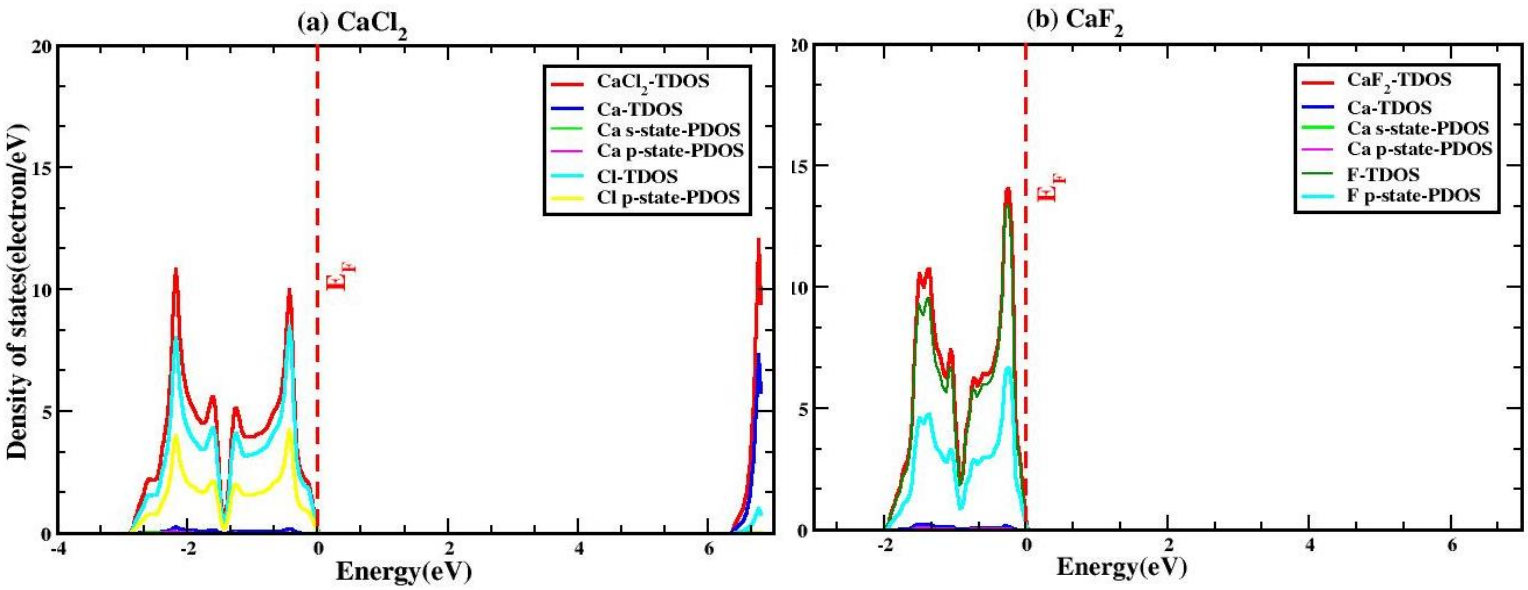

Fig 7: Density of States of $CaCl_2$ and CaF_2

Optical Properties

The dielectric behavior of $CaCl_2$ and CaF_2 is studied in the form of the real $\varepsilon_1(\omega)$ and the imaginary $\varepsilon_2(\omega)$ components of the complex dielectric function across a large photon energy spectrum, which gives an understanding of the optical polarization and absorption properties of these materials.

The real component $\varepsilon_1(\omega)$ is the dispersive behavior of the materials. Both of $CaCl_2$ and CaF_2 have positive and high values of $\varepsilon_1(\omega)$ (in the static limit) at low photon energies (0-5 eV), suggesting strong polarization and dielectric response of both materials. $CaCl_2$ has a higher initial dielectric constant, and peaks at about ~6 -7 at 7-8 eV, compared to a relatively lower value of ~4 -5 at 10-11 eV in CaF_2. As the energy of the photon (10-20 eV) becomes larger, the value of $\varepsilon_1(\omega)$ of both materials becomes smaller, indicating a lower polarizability since interband transitions start to occur. It is notable that, at the high-energy region (approximately 25-30 eV), the $\varepsilon_1(\omega)$ value of both compounds decreases drastically and becomes negative, indicating that in this energy range, plasma resonance and metallic-like reflective behavior occurs. At higher photon energies, above 30 eV, $\varepsilon_1(\omega)$ tends to zero and levels off, implying reduced dispersion at higher photon energies.

The optical absorption due to interband electronic transitions is characterized by the imaginary part $\varepsilon_2(\omega)$. At low energy (below 5 eV), both materials have $\varepsilon_2(\omega)$. almost equal to zero, which validates that they are wide band gap insulating materials with no low-energy electronic excitations. With higher photon energy, there are prominent absorption peaks caused by transitions between halogen p-states in the valence band and Ca-derived conduction band states. In the case of $CaCl_2$, the significant peaks are found in the energy range of 7-15 eV with the maximum intensity found in the range of 8-10 eV, and other smaller features which extend to 20 eV. Conversely, CaF_2 shows its main absorption peak at a bit higher energies (~10-12 eV), then a strong and sharp peak at a bit higher energies (~ 28-30 eV), which is associated with higher-energy interband transitions and more localization of F-p states. The general tendency of peaks to increase in energy in CaF_2 is also in line with the larger band gap of this compound.

At higher energies (>30 eV), $\varepsilon_2(\omega)$ of both materials decreases and tends to zero, which means that there is less optical absorption and the interband transitions available have been exhausted. The spectral properties of both $\varepsilon_1(\omega)$ and $\varepsilon_2(\omega)$ confirm that CaF_2 has a higher high-energy optical response, and a larger band gap, whereas $CaCl_2$ has a relatively high degree of low-energy polarizability.

In general, the dielectric properties of the two compounds are typical of wide band gap ionic insulators, with unique energy-dependent polarization and absorption characteristics. These

characteristics enable them to be used in optical coatings, UV-transparent materials, and high-frequency dielectric devices, especially CaF_2, because it has a better performance in the high-energy (ultraviolet) region.

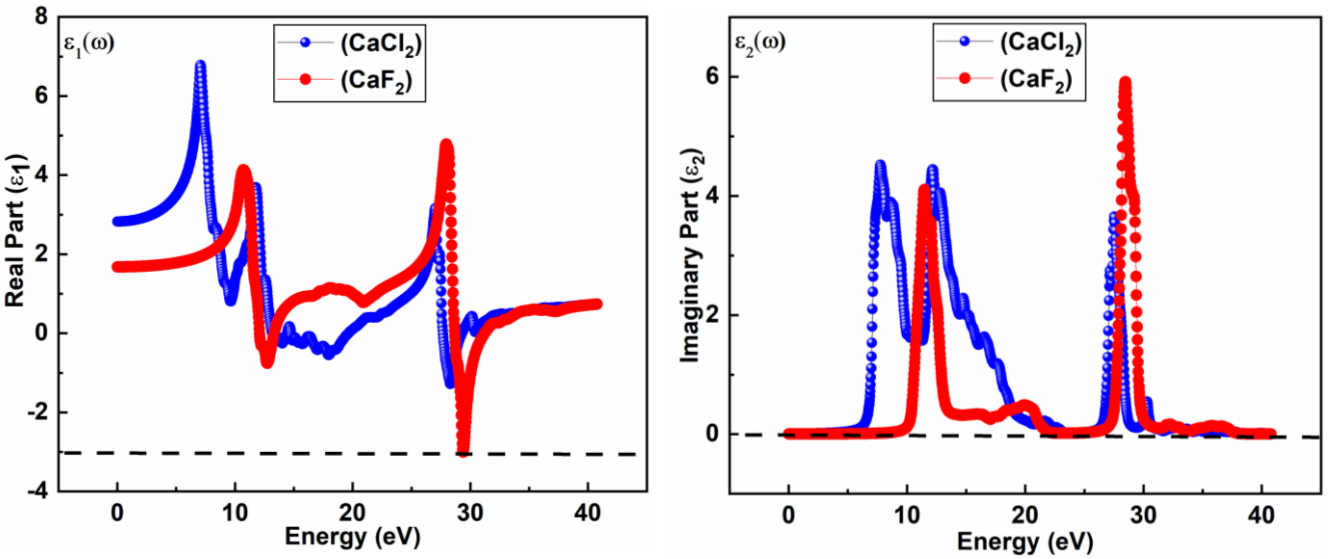

Fig 8: Real (ε_1) and imaginary (ε_2) parts of the dielectric function for $CaCl_2$ and CaF_2

The optical characteristics of $CaCl_2$ and CaF_2 were studied in a systematic way over a photon energy range, and showed characteristic properties of wide band-gap insulating materials. Both compounds have the optical conductivity negligible at low energy implying the lack of free charge carriers and sharply increases at high energy, as a result of interband electronic transitions. It is important to note that the peaks of conductivity of CaF_2 are much higher than those of $CaCl_2$, which implies that the electronic excitation is stronger at higher photon energies.

This can be seen in the absorption coefficient spectra, where both materials exhibit onset absorption exceeding their band-gap energies, after which the materials exhibit strong peaks in the ultraviolet. CaF_2 absorption profile is sharper and stronger, which means that it is better able to absorb high-energy photons, and $CaCl_2$ absorption features are broader and occur at a broader energy range.

The reflectivity spectra also substantiate this change of the transparent character of both materials in the low-energy (visible) region with reflectivity rising significantly in the ultraviolet region. CaF_2 exhibits more reflectivity peaks, which means that it interacts more with incident electromagnetic radiation.

The analysis of the refractive indices shows that $CaCl_2$ has a relatively higher refractive index at lower energies indicating a greater polarization response although both materials have anomalous dispersion at resonance energies. In the low-energy region, the extinction coefficient of both compounds is near zero, which indicates that there is minimal absorption, but it rises sharply with energy, with the CaF_2 once again exhibiting stronger peaks.

Further, the energy loss function shows discrete plasma resonance peaks, at 28-29 eV with $CaCl_2$ and slightly bigger, at 30-31 eV with CaF_2. The sharper and more intense peak in CaF_2 indicates stronger collective oscillations of the electron plasma. In general, the comparative analysis shows that both $CaCl_2$ and CaF_2 are optically inactive in the visible and active in the ultraviolet range; however, CaF_2 always shows stronger optical responses to all the parameters studied. This implies that CaF_2 should be used in high-energy optical and ultraviolet applications whereas $CaCl_2$ has relatively moderate and broad optical behavior.

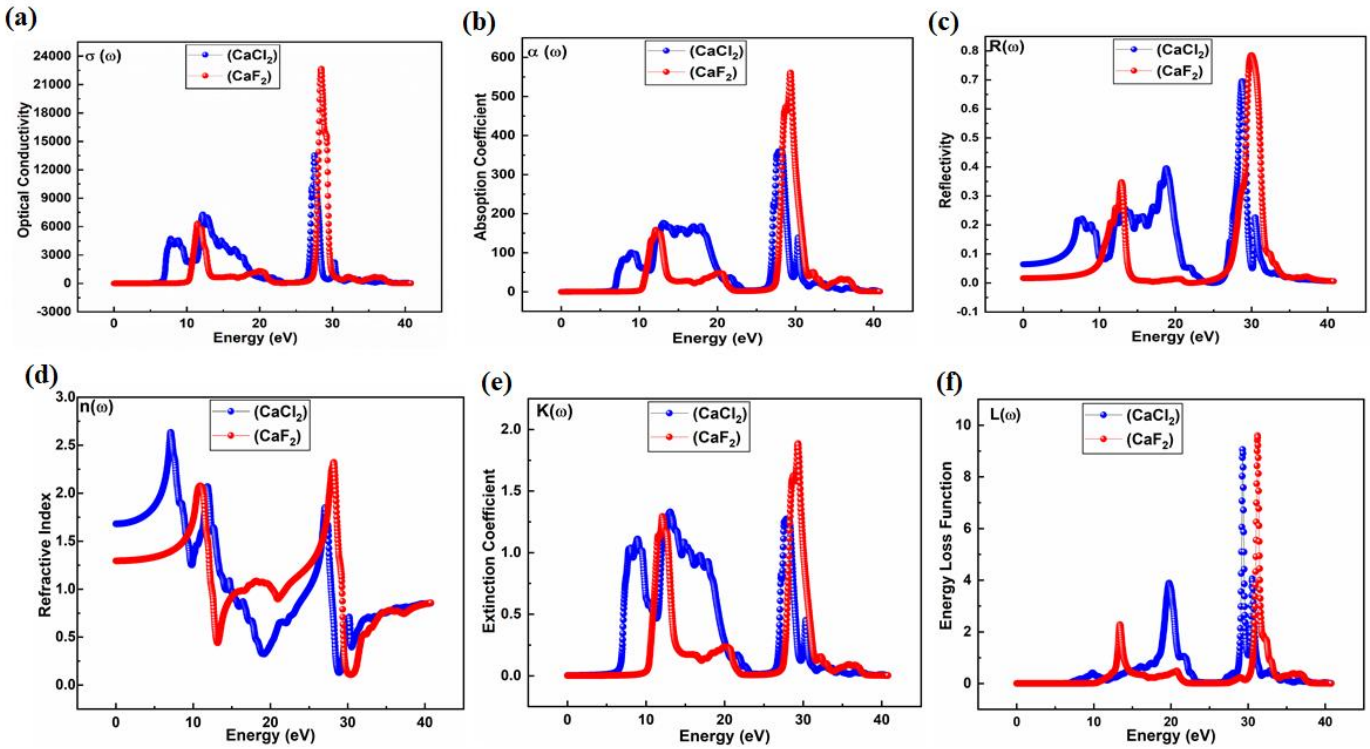

Fig 9: The Optical Conductivity (a); Absorption Coefficient (b); Reflectivity R(ω) (c); Refractive Index n (ω)(d); Extinction Coefficient K(ω) (e); and Energy Loss Function L(ω)(f) $CaCl_2$ and CaF_2.

Conclusion

The structural, mechanical, electronic and optical properties of $CaCl_2$, CaF_2 have been investigated in this work through the detailed analysis of these compounds using DFT. Structural results verify that both materials are cubic phase and CaF_2 has higher structural rigidity, as a result of the higher bulk modulus. Elastic characteristics demonstrate that both of the compounds meet the requirements of mechanical stability, but CaF_2 is determined to be mechanically stronger, stiffer and ductile, and $CaCl_2$ is relatively soft and brittle. The anisotropy test also reveals that the two materials are elastic anisotropic materials with $CaCl_2$ having a higher directional dependence.

Calculations of electronic structure establish that both $CaCl_2$ and CaF_2 are indirect wide band gap insulators, CaF_2 has a larger band gap owing to increased ionic character and local F-p states. Optical analysis shows that the two materials are both transparent in the visible region and strongly absorb and are optically active in the ultraviolet region. Remarkably, the optical responses of CaF_2 are more intense and sharper, reflective and have stronger plasma resonance peaks, which makes it more applicable to high-energy optical applications.

Comprehensively, the comparison analysis determines CaF_2 as an excellent material in mechanical strength and optical performance especially in ultraviolet and high-frequency applications of dielectric, and it might find application where lower stiffness and moderate optical performance are needed. The results can be very useful to the design and implementation of the wide band gap materials in the advanced optoelectronics and photonic devices.

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