Insights into the physical properties of a $CaCuO_3$ and $SrCuO_3$ semi-metals: A DFT study

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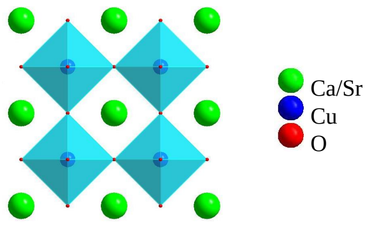
Introduction



Two dimensional view of $CaCuO_3$

Lattice constant and unit cell volume

Compound	*a* (Å)	V(Å³)	Ref.
$CaCuO_3$	3.804	55.05	This
$SrCuO_3$	3.884	58.60	This

$ACuO_3$ (A=Ca, Sr) type perovskite are of great interest due to their potential technological importance in sectors including dielectrics, photovoltaics, subtracts for superconducting materials and optoelectronics [1,2]. Nowadays, $ACuO_3$ (A=Ca, Sr) perovskites are attracting the attention of the scientist community due to their catalytic and superconducting properties.

Target of the study: **Investigation of Structural, elastic, electronic and optical properties of $ACuO_3$ (A=Ca, Sr) .**

Methodology

- First Principle Calculations
- Pseudopotential Method
- DFT theory
- GGA

CASTEP code

Optimized Structure

Characterization

- Structural, electronic, elastic, and optical properties without and with pressure
- Superconducting temperature

Plane-wave cut off energy = 450 eV
Monkhorst-Pack grid = 15×15×15
Pseudopotential: Ultrasoft

Valence orbitals:
Sr- $4s^2$, $4p^6$, $5s^2$; Ca-$3s^2$ $3p^6$, $4s^2$
Cu-$3d^{10}$, $4s^1$; O-$2s^2$, $2p^4$

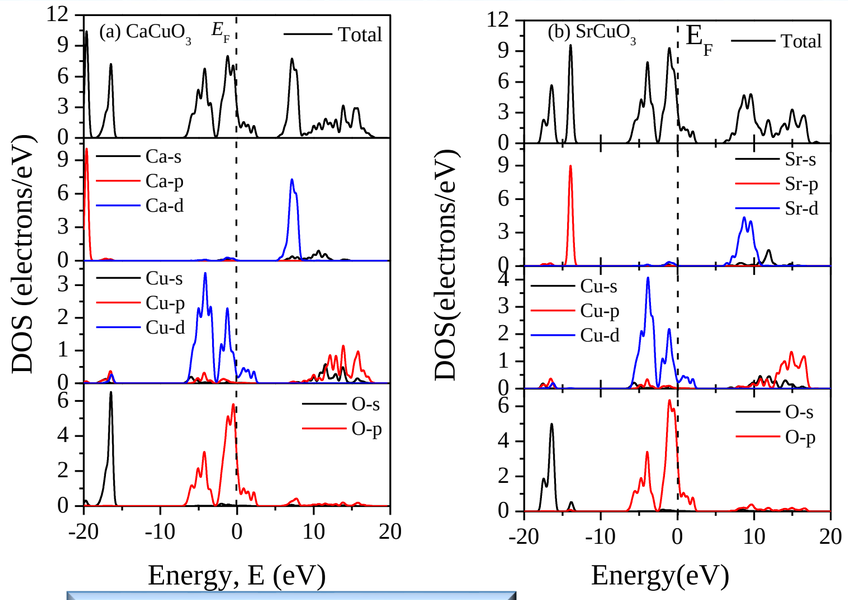
Results and Discussion

Elastic Properties

Table 1: Calculated independent elastic constants (C_{ij}, in GPa), Bulk Modulus (B, in Gpa), share modulus (G, in GPa) and Poisson's ratio (υ).

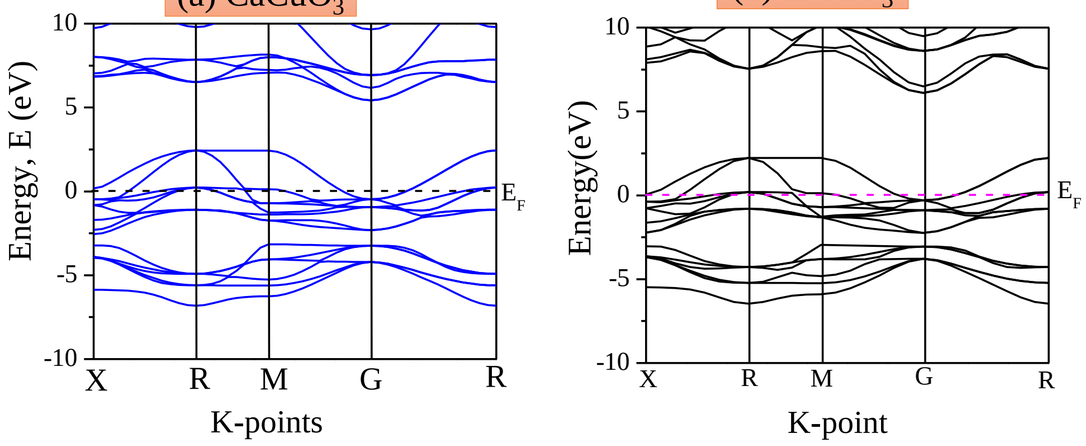
Compound	C_{11}	C_{12}	C_{44}	B	G	υ
$CaCuO_3$	232.7	88.9	42.9	136.8	56	0.32
$SrCuO_3$	212.8	84.2	54.3	127.1	62.8	0.29

- Satisfy stability criteria
- Ductile nature
- Suitable for thermal coating
- Mixed ionic-covalent bonding.



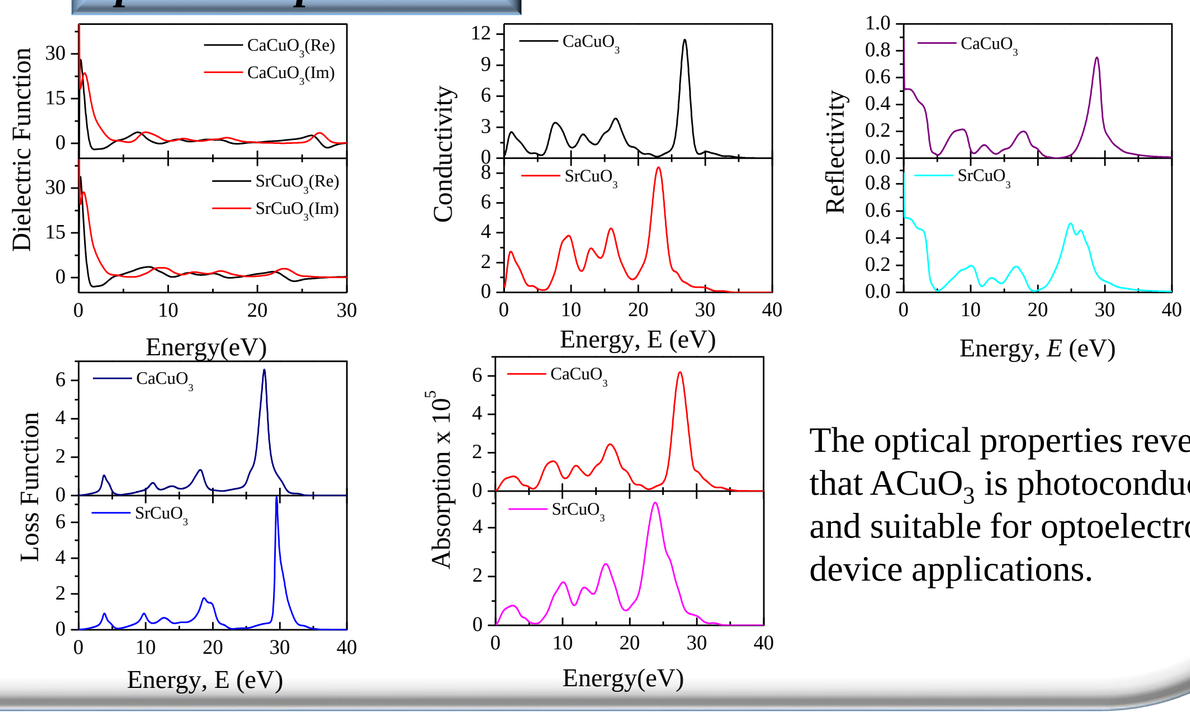
For both the compounds, near the Fermi level strong hybridization occurs between *d* and *p* orbitals of Cu and O atoms, respectively.

Electronic Properties



For both the compounds, valence band crosses the Fermi level, which suggests the metallic character of $ACuO_3$. The distance between X-R and R-M is not the same which reflects the anisotropic character.

Optical Properties



The optical properties reveal that $ACuO_3$ is photoconductive and suitable for optoelectronic device applications.

Conclusions

The mechanical stability is proved from the elastic constants. The band structure calculations disclose the metallic nature where Cu-3*d* and O-2*p* levels are dominated at the Fermi level. The high values of absorption coefficient and reflectivity are found in the UV region. .

References

[1] T. Ishihara, *Springer Handbook of Electronic and Photonic Materials*, DOI 10.1007/978-3-319-48933-9_59.
[2] E. A. R. Assirey, Saudi Pharm. J. **27**, 817 (2019).