Ab initio study on structural, elastic, electronic and optical properties of cuprate based superconductor

Uttam Kumar Chowdhury1, Md. Atikur Rahman1*, Md. Afjalur Rahman1, M.T.H. Bhuiyan1 and Md. Lokman Ali1

Abstract: The structural, elastic, electronic, and optical properties of BaCuO2 are investigated using the plane-wave ultrasoft pseudo-potential technique, which is based on the first-principle density functional theory (DFT) with generalized gradient approximation (GGA). The calculated structural parameters show a good agreement with the experimental and other theoretical results. The optimized lattice parameters, independent elastic constants ($C_{11}$, $C_{12}$, $C_{13}$, $C_{33}$, $C_{44}$ and $C_{66}$), Bulk modulus B, compressibility K, Shear modulus G, and Poisson's ratio $\nu$, as well as the band structures, total and atom-projected densities of states and finally the optical properties of BaCuO2 has been evaluated and discussed. The band structure and density of states show that these phases have metallic behavior and the major contribution comes from O-2P states for BaCuO2. Further, the first time investigated optical functions reveal that the reflectivity is high in the IR-UV region up to 28.5eV for BaCuO2 respectively, showing this to be a promising coating material.

1. Introduction
The phenomenon of superconductivity has a rich and interesting history, starting in 1911 when Kamerlingh Onnes discovered that upon cooling elemental mercury to very low temperatures, the electrical resistance suddenly and completely vanished below a critical temperature $T_c$ of 4 K (−452°F) (Timmer, 2011). This resistanceless state enables persistent currents to be established in circuits to

ABOUT THE AUTHORS
Md. Atikur Rahman’s research group studies to investigate different properties such as elastic, electronic, optical, and thermodynamic properties of materials at ambient condition and under pressure. All the calculations performed using the density functional theory (DFT) based CASTEP computer program together with the generalized gradient approximation (GGA) with the PBE exchange-correlation function. We have also prepared crystalline powder by solid-state reaction technique using carbolite furnace. The composition and crystalline phase will be confirmed by the X-ray powder diffraction (XRD). We will also synthesize the single crystals of oxide materials by Bridgman method using modified horizontal Bridgman furnace.

PUBLIC INTEREST STATEMENT
We have investigated the structural, elastic, electronic, and optical properties of BaCuO2 using the plane-wave ultrasoft pseudo-potential technique, which is based on the first-principle density functional theory (DFT) with generalized gradient approximation (GGA). To the best of our knowledge, this is the first quantitative theoretical prediction of the electronic, elastic, and optical properties of this superconducting compound. We hope that this technique will help to investigate the different properties of other superconducting materials.
generate enormous magnetic fields, and to store and transport energy without dissipation. Superconductors have other unique properties such as the ability to expel and screen magnetic fields, and quantum oscillations controlled by the magnetic field that provide extraordinary measurement sensitivity. Due to the very low operating temperature, the practical applications of conventional superconductors are limited. Over the intervening years, the number of superconducting materials has grown, with higher critical temperatures and improved metallurgical properties, and these have found their way into a number of technological applications such as MRI imaging systems for the health care industry, Josephson devices, Superconducting Quantum Interference Devices (SQUID), Magneto encephalography, microwave devices and resonators to high energy physics experiments. The high-temperature superconductivity of cuprates (“kings” of superconductors) was discovered in 1986 by Georg Bednorz and Alex Müller, when the highest superconducting transition temperature (i.e. critical temperature) characteristic of conventional superconductors ($T_c = 23.2$ K in Nb$_3$Ge) substantially exceeded and a superconducting transition temperature $T_c = 30$ K was achieved in the ceramic La$_{2-x}$Ba$_x$CuO$_{4-δ}$ (Bednorz & Müller, 1986). Today, the material HgBa$_2$Ca$_2$Cu$_3$O$_{8+δ}$ that becomes superconducting at the highest temperatures: $-135$°C or 138 K. However, the origin of their superconductivity has not been found yet and remains one of the most important and difficult mysteries of modern physics. Yet, cuprates' composition and structure is quite simple: they are composed of piled up atom layers. In all cuprates, we find copper and oxygen layers with a square structure.

The number of electrons in these layers can be modified by oxidizing the material or modifying its chemical composition; this is called “doping.” At present, there are more than 150 superconducting compounds with $T_c$ higher than the record of 23 K for conventional superconductors but only cuprates can be called the true high-temperature superconductors since only they have $T_c$ above the liquid nitrogen boiling point and many of them even have $T_c > 100$ K. However, for practical application of superconductors, we need superconductors with higher critical temperature and cuprate is best for this. During the past decade, remarkable progress in the areas of basic research and technological applications has been made on the high $T_c$ cuprate superconductors. The availability of high-quality polycrystalline materials, single crystal bulk, and thin film materials has made it possible to make reliable measurements of the physical properties of these materials and to optimize superconducting properties (e.g. $J_c$) that are important for technological applications. In this work, our investigations have provided important information regarding the structural, elastic, electronic and as well as the optical properties of this superconductor. The next decade of research on the high $T_c$ cuprate superconductors as well as other novel superconducting materials promises to yield significant advances toward the development of a theory of high-temperature superconductivity as well as the realization of technological applications of these materials on a broad scale. It is possible that significantly higher values of $T_c$ will be found in new cuprate compounds or other classes of materials. In this research paper, we have studied the structural, electronic, elastic, and optical properties of iron and cuprate-based superconductors of BaCuO$_2$ using plane-wave pseudopotential density functional theory method (DFT) with generalized gradient approximation (GGA). The remaining parts of this paper are organized as follows. In Section 2, the computation details are given. The results and discussion are presented in Section 3. Finally, a summary of our results is shown in Section 4.

2. Computational method

The first-principle investigations were carried out using the plane-wave pseudo-potential method based on the density functional theory (Kohn & Sham, 1965) implemented in the CASTEP code (Clark et al., 2005). The exchange-correlation energy is treated within the GGA using Perdew–Burke–Ernzerhof (PBE) scheme (Perdew, Burke, & Ernzerhof, 1996). The ultrasoft pseudo-potentials were used in the calculations, and the plane-wave cut-off energy was used 350 eV. For the sampling of the Brillouin zone a Monkhorst-Pack grid (Monkhorst & Pack, 1976) of $10 \times 10 \times 12 k$-points were used for BaCuO$_2$. The equilibrium crystal structures are obtained via geometry optimization in the Broyden–Fletcher–Goldfarb–Shanno (BFGS) minimization scheme (Fischer & Imlof, 1992). Geometry optimization was performed using the total energy of $1 \times 10^{-5}$ eV/atom, maximum force of
0.002 eV/Å, maximum stress of 0.05 GPa, and the maximum atomic displacement of $1 \times 10^{-3}$ Å. Mulliken bond population, electronic density of states (EDOS), elastic constants $C_{ij}$, and optical properties were directly calculated using the CASTEP code.

3. Results and discussion

3.1. Structural properties

The cuprate-based superconductor BaCuO$_2$ belongs to tetragonal structure with the space group $P4/mmm$ (No. 123). The equilibrium lattice parameters have a value of $a = 3.93$ Å and $c = 3.47$ Å. The lattice constants and atomic positions have been optimized as a function of normal stress by minimizing the total energy. The optimized structure is shown in Figure 1. The calculated values of the structural properties of BaCuO$_2$ are presented in Table 1 along with the available experimental values. From Table 1, we see that our present theoretical results are almost close to experimental results. The calculated lattice constant of this present work are 4.071 and 3.823 Å which show 3.58 and 10.17% deviation compared with the experimental values due to the different calculation methods. The existing discrepancy can be attributed to the fact that our calculated data are simulated at 0 K, while the experimental data are measured at room temperature. This indicates the reliability of our present DFT-based first-principle calculations.

3.2. Elastic properties

The elastic properties of materials provide useful information about the bonding character between adjacent atomic planes, the anisotropic character of the bonding, the structural stability, and the stiffness of materials. These properties also provide the information about the interatomic potentials, interatomic bonding, thermal expansion, Debye temperature, phonon spectra, and specific heat capacity (Bouhemadou, Khenata, Chegaar, & Maabed, 2007; Pan, Xia, Ye, & Ding, 2012; Ponce, Casali, & Caravaca, 2008). Elastic constants are defined by means of a Taylor expansion of the total energy, namely the derivative of the energy as a function of a lattice strain (Clark et al., 2005; Perdew & Zunger, 1981). In order to study the elastic properties of BaCuO$_2$, the elastic constants $C_{ij}$, Bulk modulus $B$, Shear modulus $G$, Young’s modulus $E$, Poisson’s ratio $\nu$, and the anisotropic factor $A$ has been calculated for the first time and are presented in Table 2. The tetragonal

![Figure 1. The crystal structures of BaCuO$_2$, (a) the conventional cubic cell and (b) the primitive cell.](image)

| Compound  | Lattice parameters (Å) | Unit cell volume V ($\text{Å}^3$) | Bulk modulus B (GPa) | Atomic positions | Deviation from Expt. in % | Ref. |
|-----------|------------------------|----------------------------------|----------------------|------------------|--------------------------|-----|
| BaCuO$_2$ | $a = 4.071, 3.930^*$    | 63.35                            | 116.88               | Ba (0.5, 0.5, 0.5) | 3.58                      | Present |
|           | $c = 3.823, 3.470^*$    |                                  |                      | Cu (0, 0, 0)      | 10.17                     |      |
|           |                        |                                  |                      | O (0, 0.5, 0)     |                          |      |

*Experimental value (Gómez et al., 2010).
Crystal like \( \text{BaCuO}_2 \) has six independent elastic coefficients \( C_{ij} \), i.e., \( C_{11}, C_{12}, C_{13}, C_{33}, C_{44} \) and \( C_{66} \). At present, no experimental data are available because of first time study. For a stable tetragonal structure, the six independent elastic constants \( C_{ij} \) should satisfy the following Born–Huang criteria (Roknuzzaman & Islam, 2013):

\[
\begin{align*}
C_{11} > 0; & \quad C_{33} > 0; \quad C_{44} > 0; \quad C_{66} > 0 \\
(C_{11} - C_{12}) > 0; & \quad (C_{11} + C_{33} - 2C_{13}) > 0 \\
2[(C_{11} + C_{12}) + C_{33} + 4C_{13}] > 0
\end{align*}
\]

The calculated elastic constants presented in Table 2 are positive and satisfy the above conditions. This suggests that these superconductors are mechanically stable compounds. The elastic anisotropy of a crystal is the orientation dependence of the elastic moduli or sound velocities. A proper description of such an anisotropic behavior has an important implication in engineering science as well as in solid state (crystal) physics. To quantify the elastic anisotropy of tetragonal structures, \( \text{BaCuO}_2 \), we have evaluated Zener anisotropic factor defined by

\[
A = \frac{C_{44}}{(C_{11} - C_{12})}
\]

The calculated Zener anisotropic factor of \( \text{BaCuO}_2 \) is presented in Table 2. The Zener anisotropy factor \( A \) is used for measuring the degree of elastic anisotropy in solids. The value of \( A = 1 \) for a completely isotropic material and if \( A \) is smaller or greater than one, it shows that the material is anisotropic. As shown in Table 2, the value of \( A \) for \( \text{BaCuO}_2 \) is larger than unity, indicating that the material under studied can be regarded as elastically anisotropic material. Another anisotropy parameter defined by the ratio between linear compressibility coefficients along the c and a axis for tetragonal crystal is

\[
k_c/k_a = (C_{11} + C_{12} - 2C_{13})/(C_{33} - C_{13})
\]

Our result reveals that the compressibility along the c axis is slightly larger than that along the a axis. This factor also indicates that the material \( \text{BaCuO}_2 \) is anisotropy.

We have estimated the Bulk modulus (\( B \)) and Shear modulus (\( G \)) of polycrystalline aggregates from individual elastic constants, \( C_{ij} \), by the well-known Voigt (Monkhorst & Pack, 1976) and the Reuss (1929) approximations that are recurrently used in averaging the single-crystal elastic constants for polycrystalline manners. Voigt assumes the uniform strain throughout a polycrystalline aggregate and Reuss assumes the uniform stress. The Bulk modulus \( B_V \) and Shear modulus \( G_V \), in the Voigt approximation for the tetragonal lattice are expressed as:

\[
B_V = \frac{1}{9} \left[ 2(C_{11} + C_{12}) + 4C_{13} + C_{33} \right]
\]

\[
G_V = \frac{1}{30} \left( C_{11} + C_{12} + 2C_{33} - 4C_{13} + 12C_{44} + 12C_{66} \right)
\]

In the Reuss approximation, the Bulk modulus \( B_R \) and Shear modulus \( G_R \) are expressed as:

\[
B_R = \frac{(C_{11} + C_{12})C_{33} - 2C_{13}^{\prime} - C_{33}^{\prime}}{C_{11} + C_{12} + 2C_{33} - 4C_{13}^{\prime}}
\]

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Table 2. The calculated elastic constants \( C_{ij} \) (in GPa), the shear anisotropic factors \( A \), and \( k_c/k_a \) of cuprate-based superconductor \( \text{BaCuO}_2 \).

| Compound  | \( C_{11} \) | \( C_{12} \) | \( C_{13} \) | \( C_{33} \) | \( C_{44} \) | \( C_{66} \) | \( A \) | \( k_c/k_a \) | Ref. |
|-----------|-------------|-------------|-------------|-------------|-------------|-------------|------|------------|------|
| \( \text{BaCuO}_2 \) | 148         | 85          | 41          | 145         | 46          | 66          | 1.460| 1.45       | Present |


\[
G_R = \frac{5C_{44}C_{66} \left[ (C_{11} + C_{12})C_{33} - 2C_{13}^2 \right]}{2 \left[ 3B_V C_{44}C_{66} + \left\{ (C_{11} + C_{12})C_{33} - 2C_{13}^2 \right\} (C_{44} + C_{66}) \right]}
\]

(7)

It is evident that the Voigt and Reuss assumptions are true only for isotropic crystals, but for an anisotropic crystal their assumptions become immediately invalid. Hill (1952) showed that for anisotropic crystals the Voigt and Reuss assumptions result in theoretical maximum and minimum values of the isotropic elastic moduli of the polycrystalline crystals, respectively, and suggested that the actual effective moduli of anisotropic polycrystalline crystals could be approximated by the arithmetic mean of the two values. According to Hill approximation, the Bulk modulus \( B \) and Shear modulus \( G \) are given by:

\[
B = \frac{1}{2} (B_R + B_V) \quad \text{and} \quad G = \frac{1}{2} (G_R + G_V)
\]

(8)

Again, from the calculated Bulk modulus \( B \) and Shear modulus \( G \) we can estimate the Young’s modulus \( Y \) and Poisson’s ratio \( \nu \) by the following relations:

\[
Y = \frac{9BG}{3B + G} \quad \text{and} \quad \nu = \frac{3B - 2G}{2(3B + G)}
\]

(9)

Using Equations (4)–(9) the calculated Bulk modulus \( B_R, B_V, B \), Shear modulus \( G_R, G_V, G \), Young’s modulus \( Y \), compressibility \( K \), and Poisson’s ratio \( \nu \) are listed in Table 3. It is seen that the difference between \( B_R \) and \( B_V \) as well as \( G_R \) and \( G_V \) is comparatively small. According to Hill, the difference between these limiting values may be proportional to the degree of elastic anisotropy of crystal. According to Pugh’s criteria (Pugh, 1954), a material should be brittle if its \( G/B > 0.5 \), otherwise it should be ductile. From our calculations we see that \( G/B > 0.5 \), hence the material BaCuO₂ should behave in a brittle manner. The knowledge of the Young’s modulus and Poisson’s ratio are very important for the industrial and technological applications. The Young’s modulus provides useful information about the measure of the stiffness of the solids, i.e. the larger the value of \( Y \), the stiffer the material. The Poisson’s ratio provides the information about the characteristics of the bonding forces. For covalent materials, the values of \( \nu \) are typically 0.1–0.25 and interatomic forces are non-central forces. Also, the lower and upper limits of \( \nu \) are 0.25 and 0.5 for ionic crystals and the interatomic forces are central forces. The Poisson’s ratio for a brittle material is very small, whereas for a ductile metallic material it is typically 0.33 (Clark et al., 2005). In our case, this value is smaller than 0.33 so that the material BaCuO₂ possesses the property of brittleness.

### 3.3. Electronic properties

The density of states (DOS) plays vital role in the analysis of the physical properties of materials. In solid-state and condensed matter physics, the DOS of a system describes the number of states per interval of energy at each energy level that are available to be occupied. A high DOS at a specific energy level means that there are many states available for occupation. A DOS of zero means that no states can be occupied at that energy level. The total DOS is written as a sum over atomic contributions. The DOS is calculated using the following expression

\[
N(\epsilon) = 2 \sum_{n,k} \delta \left( \epsilon - \epsilon_n^k \right) = \left( 2/V_{BZ} \right) \sum \delta \left( \epsilon - \epsilon_n^k \right) dk
\]

(10)

and the number of electron in the unit cell is given by

| Compound   | \( B_R \) | \( B_V \) | \( B \) | \( G_R \) | \( G_V \) | \( G \) | \( Y \) | \( K \) | \( G/B \) | \( \nu \) | Ref.   |
|------------|-----------|-----------|--------|----------|----------|-------|------|-----|-------|-------|-------|
| BaCuO₂     | 84.74     | 86.11     | 85.43  | 55.09    | 56.76    | 55.93 | 45.91| 0.022| 0.655 | 0.231 | Present |
Here, we perform an analysis for the electronic band structure of BaCuO$_2$. We illustrate the investigated partial density of states (PDOS) and total density of states (TDOS) at normal pressure. The calculated electronic band structure of BaCuO$_2$ along the high symmetry directions in the Brillouin zones is shown in Figure 2. The partial and total densities of states of BaCuO$_2$ are shown in Figures 3 and 4. Here, we have treated Ba-5p$^6$6s$^2$, Cu-3d$^{10}$4s$^1$, O-2s$^2$2p$^4$ as valence electrons. From Figure 2,

$$\int_{-\infty}^{\infty} n(\epsilon) \, d(\epsilon)$$

Figure 2. Electronic band structure of BaCuO$_2$ along high symmetry direction in the Brillouin zones.

Figure 3. Calculated partial density of states of BaCuO$_2$. 
it is noticed that the compound under study is metallic because a number of valance and conduction bands are overlapping at the Fermi level.

It is observed that the total DOS at the Fermi level for BaCuO$_2$ is 1.80 states per unit cell per eV. At the Fermi level, the DOS mainly originates from the O-2$^P$ states for this phase. This 2$^P$ contribution is responsible for the conduction properties of BaCuO$_2$. Ba does not contribute to the DOS at the Fermi level and therefore is not involved in the conduction properties. Cu has a poor contribution at the Fermi level.

3.4. Optical properties

The study of the optical functions helps to give a better understanding of the electronic structure of different materials. The optical properties of BaCuO$_2$ with different photon energies are calculated by the frequency-dependent dielectric function, $\varepsilon(\omega) = \varepsilon_1(\omega) + i\varepsilon_2(\omega)$, which is closely related to the electronic band structure. The imaginary part $\varepsilon_2(\omega)$ of the dielectric function is expressed as the momentum matrix elements between the occupied and the unoccupied electronic states and can be calculated directly using Materials Studio CASTEP manual © Accelrys (2010):

$$\varepsilon_2(\omega) = \frac{2e^2}{\Omega \varepsilon_0} \sum_{k,v,c} \left| \langle \psi_k^c | \hat{u} \cdot \vec{r} | \psi_v^c \rangle \right|^2 \delta(E_k^c - E_v^c - E)$$

where $\omega$ is the light frequency, $e$ is the electronic charge, $\hat{u}$ is the vector defining the polarization of the incident electric field, and $\psi_k^c$ and $\psi_v^c$ are the conduction and valence band wave functions at $k$, respectively. From the imaginary part $\varepsilon_2(\omega)$, the real part $\varepsilon_1(\omega)$ of the dielectric function is derived through the Kramers-Kronig relations. All the other optical properties, such as refractive index, absorption spectrum, loss function, reflectivity, and conductivity (real part) are derived from the formalism developed in Materials Studio CASTEP manual © Accelrys (2010).

Figure 5 exhibits the optical functions of BaCuO$_2$ calculated for photon energies up to 50 for polarization vector [100]. We have used a 0.5 eV Gaussian smearing for all calculations because this smears out the Fermi level, so that k-points will be more effective on the Fermi surface.

The most general property of solids is the dielectric function which modifies the incident electromagnetic wave of light. The dielectric function describes what an electric field such as an oscillating light wave does to material. It describes the polarization and absorption properties of the material. The quantity $\varepsilon_2(\omega)$ represents how much a material becomes polarized when an electric field is applied due to creation of electric dipoles in the material. The quantity $\varepsilon_2(\omega)$ represents absorption in a material. When a material is transparent, $\varepsilon_2(\omega)$ is zero; it becomes nonzero when absorption begins. Figure 5(a) illustrates the dielectric functions of BaCuO$_2$ as a function of photon energy. It is observed from Figure 5(a) that the value of $\varepsilon_2$ becomes zero at about 29 eV indicating that the material becomes transparent above 29 eV. For BaCuO$_2$, the value of the static dielectric constant is 6 indicating that this compound might be a promising dielectric material.
Figure 5. The optical functions (a) dielectric function, (b) refractive index, (c) absorption, (d) loss function, (e) reflectivity, and (f) conductivity of BaCuO$_2$ for polarization vector [100].
In optics, the refractive index of an optical medium is a dimensionless number that describes how light or any other radiation propagates through that medium. As function of photon energy, the refractive indices of BaCuO$_2$ are shown in Figure 5(b). It is obvious that the refractive index of this compound is high in the infrared region and gradually decreased in the visible and ultraviolet region.

The absorption coefficient provides important information about optimum solar energy conversion efficiency and it indicates how far light of a specific energy or wavelength can penetrate into the material before being absorbed. Figure 5(c) shows the absorption spectra of BaCuO$_2$ for the direction [100] which begin at zero photon energy due to metallic nature of these compounds. For BaCuO$_2$, the absorption spectra arise sharply up to 28 eV and the highest peaks for polarization direction [100] appear at 24 eV and then decrease drastically up to 43 eV. There is no absorption above 43 eV.

The energy loss function of BaCuO$_2$ as a function of photon energy is shown in Figure 5(d). It explains the energy loss of a fast electron traversing the material (Hossain, Ali, & Islam, 2012). It is defined by the bulk plasma frequency $\omega_p$ which occurs at $\varepsilon_2 < 1$ and $\varepsilon_1 = 0$. In the energy loss spectrum, we see that the effective plasma frequency $\omega_p$ of this phase is equal to 29 eV. Hence, the material becomes transparent when the incident photon frequency is higher than $\omega_p$.

The reflectivity spectrum of BaCuO$_2$ as a function of photon energy is shown in Figure 5(e). The reflectivity of BaCuO$_2$ starts with a value of ~0.20 decreases and then rises again to reach maximum value of ~0.65 in the energy range 25–28 eV. Hence, the material promises to be good coating material in this energy range.

The photoconductivity is an optoelectronic phenomenon in which electrical conductivity in a material increases due to the absorption of electromagnetic radiation. Since the material has no band gap as evident from band structure, the photoconductivity starts with zero photon energy as shown in Figure 5(f). BaCuO$_2$ crystal is highly electrically conductive when the incident radiation has energy within the range of ~3.5–4.5 eV. The photoconductivity and hence the electrical conductivity of the material increases as a result of absorbing photons. There is no photoconductivity when the photon energy is higher than 28 eV for BaCuO$_2$.

4. Conclusions
First-principle calculations based on DFT have been used to study the structural, electronic, elastic, and optical properties of the superconducting material BaCuO$_2$. The calculated lattice parameter of this compound is in good agreement with the experimental finding. The independent elastic constants, Bulk modulus, Shear modulus, Young’s modulus, elastic anisotropy factor are calculated for the first time. The compounds are shown to be mechanically stable, elastically anisotropic, and brittle. The calculated band structures and DOS show that BaCuO$_2$ is metallic and at the Fermi level the main contribution comes from the O. The optical properties such as dielectric function, refractive index, absorption spectrum, energy loss function, reflectivity, and photoconductivity are determined and analyzed in detail. The optical properties such as refractive index, reflectivity, and photoconductivity are found to be polarization-dependent. The reflectivity spectrum implies that BaCuO$_2$ is a potential candidate material for coating to reduce solar heating. The conductivity spectrum shows that electrical conductivity increases as a result of absorbing photons.

**Funding**
The authors received no direct funding for this research.

**Author details**
Uttam Kumar Chowdhury$^1$
E-mail: phy.uttam@gmail.com
Md. Atikur Rahman$^1$
E-mail: atik0707phy@gmail.com
Md. Afjalur Rahman$^1$
E-mail: afjal.sust36@gmail.com
M.T.H. Bhuiyan$^1$
E-mail: thbapon@gmail.com
Md. Lokman Ali$^1$
E-mail: lokman.cu12@gmail.com

$^1$Department of Physics, Pabna University of Science and Technology, Pabna 6600, Bangladesh.

**Citation information**
Cite this article as: Ab initio study on structural, elastic, electronic and optical properties of cuprate based superconductor, Uttam Kumar Chowdhury, Md. Atikur Rahman, Md. Afjalur Rahman, M.T.H. Bhuiyan & Md. Lokman Ali, Cogent Physics (2016), 3: 1231361.
