Experimental and Theoretical Studies of Green Synthesized \( \text{Cu}_2\text{O} \) Nanoparticles Using *Datura Metel L*

Karuppaiah Chinniaiah\(^1\) · Vivek Maik\(^2\) · Karthik Kannan\(^3\) · V. Potemkin\(^4\) · M. Grishina\(^4\) · M. Gohulkumar\(^5\) · Ratnesh Tiwari\(^6\) · K. Gurushankar\(^1,4\)

Received: 17 August 2021 / Accepted: 27 December 2021 / Published online: 8 January 2022
© The Author(s), under exclusive licence to Springer Science+Business Media, LLC, part of Springer Nature 2022

Abstract
In biomedical applications, \( \text{Cu}_2\text{O} \) nanoparticles are of great interest. The bioengineered route is eco-friendly for the synthesis of nanoparticles. Therefore, in the present study, there is an attempt to synthesis \( \text{Cu}_2\text{O} \) nanoparticles using *Datura metel L*. The synthesized nanoparticles were characterized by UV–Vis, XRD, and FT-IR. UV–Vis results suggest the presence of hyoscyamine, atropine in *Datura metel L*, and also, nanoparticles formation has been confirmed by the presence of absorption peak at 790 nm. The average crystallite size (19.56 nm) was obtained by XRD. FT-IR was also used to confirm the different functional groups. Fourier Power Spectrum was also employed to examine the synthesized nanomaterials spectrum data to emphasize the peak of the prominent frequencies. Density functional theory (DFT) was also utilized to assess the energy of the substance over time, which appears to indicate a stable molecule. Furthermore, calculated energies, thermodynamic properties (such as enthalpies, entropies, and Gibbs-free energies), modeled structures of complexes, crystals, and clusters, and predicted yields, rates, and regio- and stereospecificity of reactions were all in good agreement with experimental results. Overall, the results show that the successful production of \( \text{Cu}_2\text{O} \) nanoparticles with *Datura metel L* corresponds to theoretical research.

Keywords *Datura metel L* · \( \text{Cu}_2\text{O} \) nanoparticles · UV · XRD · FT-IR · DFT

Introduction
Engineered nanoparticles and their technical implications are already generating breakthrough ideas in the industrial process by leveraging optical, electrical, magnetic and biological features [1–5]. \( \text{Cu}_2\text{O} \) is an important promising candidate among the transition-metal oxides due to high abounded, nontoxic and cheap availability. Generally, it consists of (+1, +2 oxidation states known as cuprous and cupric ions [6]. The nanoparticles of \( \text{Cu}_2\text{O} \) is naturally P-type semiconductor material with a narrow bandgap of 1.2 and 2 eV, which could be favor of light absorption in several biomedical applications such as MRI-ultra sound dual imaging, microbial activity [7, 8], and bandgap of 2.98 eV used as a photoelectrode for solar energy conversion [9]. The green path to the manufacture of copper oxide nanoparticles is a simple and environmentally benign technology [10]. Hence, green synthesis is the best adopted route for nanoparticles production when compared with the chemical method due to without requirement of any reducing and stabilizing agent. The plant metabolism like flavonoid, alkaloids, terpenoids,
polyphenols, and proteins are a reservoir of plant tissue, it could be used as a reducing agent on various nanoparticles synthesis [11, 12]. *Datura metel* L. is a Solanaceae family agriculture plant that is geographically spread over on gibbous world either as an origin or foreign plant in Asia, America, and Europe. The species of *Datura metel* L. have been used as classical Chinese medicine for the treatment of asthma, coughs and antitumor activities, etc. Particularly, the major constituent of this plant namely withanolides having plant steroids built on by ergostane skeleton in the side chain of δ-lactone and their predominant alkaloid content of hyoscyamine, atropine has given the medicinal properties on nanoparticles formulation [13]. Various experimental studies show that the size and morphology of Cu$_2$O nanoparticles play an important role in the appearance of specific properties [14–17]. For example, nanocubic Cu$_2$O particles can reduce CO$_2$ emissions in the gas phase through the possibility of performing heterogeneous photocatalytic hydrogenation [14]. Smaller cubic Cu$_2$O nanoparticles exhibit the strongest gas-sensitive response [15]. It is known that the cabbage-like architecture of Cu$_2$O makes it possible to form nanocomposites with various substances, in particular with graphene oxide [16]. The nanocomposites are used for photocatalysis to remove organic pollutants by exposure to sunlight [16, 17]. It is also known that the use of organic substances, their combinations, and plants in the synthesis of nanoparticles makes it possible to create a structure of nanocomposites with a well-defined morphology [17]. In particular, the addition of glucose leads to an increase in the size of nanoparticles with a cabbage-like architecture [16, 17]. By varying the choice of plant, the concentration of the extract for green synthesis of nanoparticles, it is possible to achieve the formation of nanoparticles of the required size and shape. For example, Ramesh et al. [18] obtained spherical and hemispherical Cu$_2$O nanoparticles using the leaf extract of Arachis hypogea L. Abboud et al. [19] also synthesized spherical Cu$_2$O nanoparticles using Bifurcaria bifurcate, a marine alga. Kerur et al. [20] received truncated octahedron, octahedral and spherical Cu$_2$O nanoparticles, simply by varying the concentration of the Aloe vera leaf plant extracts. Thus, using new plants and varying the concentration of their extract, Cu$_2$O nanoparticles with a specific structure and unique properties can be obtained. In this regard, it is necessary to study new ways of green synthesis of Cu$_2$O nanoparticles.

DFT has been used for understanding and studying the stability of new compounds in previous documents [21, 22]. Using a general approximation gradient (GGA) and the interpolation method [23], the electron exchange and correlation of geometry optimization, electronic structure, and optical properties were determined. The interaction between the electron and the ion is defined by an ultra-soft potential provided by the Vanderbilt optimization approach. The electronic valence wave properties are extended to a 16 eV power reduction on a plane wave basis. Fourier power values, in addition to DFT, can be utilized to determine the indigenous signature of any substance [24, 25]. The four spectral selections are different for different compounds and the same for the same molecules. Studying the pureness, stability and other intrinsic characteristics of the compound, which can be directly seen at the peaks of Fourier, can benefit us. Therefore, there is an attempt to synthesize Cu$_2$O nanoparticles using *Datura metel* L. in the current research. UV–Vis, XRD, and FT-IR were used to characterize the synthesized nanoparticles and further the compound stabilization has calculated by the DFT method. Calculated energies, thermodynamic properties (such as enthalpies, entropies, and Gibbs-free energies), modeled structures of complexes, crystals, and clusters, and anticipated yields, rates, and regio- and stereospecificity of reactions are also investigated.

**Experimental**

**Materials & Methods**

The homogeneous *Datura metel* L. leaves collected from farmland on Krishnankoil, Tamil Nadu, India and Copper nitrate (Cu(NO$_3$)$_2$) purchased from SRL chemicals Mumbai, India, used without any further purification for the synthesis of Cu$_2$O nanoparticles. *Datura metel* L. leaves dried at room temperature up to brown after then grained by mortar and pestle. The prepared powder was consumed for all the characterization and double distilled (DD) water was used throughout the experiment.

Dust and organic moieties in leaves of *Datura metel* L. were cleaned through the process of washing in tap water followed by DD water after then leaves were cut into small pieces. 10 mg of leaves poured into the 100 ml of DD water boiled at 60 °C for 20 min in a magnetic stirrer with a speed of 70 rpm. After cooling, the prepared extract solution has filtered through the Whatman No.1 filter paper. This extract was used as a reducing agent in copper oxide nanoparticles (Cu$_2$O NPs) synthesis.

In this experiment, 20 ml of extract was added drop by drop with 100 ml of 3 mM copper nitrate aqueous solution. The reaction mixture of copper nitrate and leaf extract stirrer for 20 min in this meantime the colour of the solution changed from blue to sea green, which indicates the formation the Cu$_2$O NPs. The formed NPs are maintaining the room temperature up to 15 days after that start to obtain black precipitation. The prepared NPs are filtered and dried at 60 °C for 3 h.
Characterization

The UV–Vis absorption spectra are recorded on Shimadzu UV–1800 suited with 10 mm quartz cuvette. XRD measurements were carried out on Bruker Eco D8 Advance diffractometer with Cu-Kα radiation (λ = 1.54060 Å). FTIR analysis was performed at room temperature on IRTracer-100 Shimadzu.

Results and Discussion

Spectral Characterization

The Born–Oppenheimer approximation describes an inhomogeneous electron gas as a collection of interacting point electrons traveling quantum–mechanically in the potential domain of a set of static atomic nuclei. The independent electron approximation, Hartree theory, and Hartree–Fock theory are the most common approximation schemes used to solve such models. However, over the last thirty years or so, another approach-DFT-has become increasingly popular for the solution of such problems. This approach has the advantage of being able to solve a wide variety of problems with high precision while still being computationally simple. The electronic structure of atoms, molecules, and solids can be measured using DFT. Its goal is to get a quantitative understanding of material properties by using quantum mechanics’ fundamental laws.

The Schrödinger equation of N interacting electrons traveling in an external, electrostatic potential is solved using classic electronic structure methodologies (typically the Coulomb potential generated by the atomic nuclei). This approach, however, has two important drawbacks: (1) the problem is nontrivial even for small N, and the resulting wave functions are sophisticated objects; and (2) the computational effort grows exponentially with N, making the description of bigger systems unaffordable. DFT provides a distinct approach, focusing on the one-body density rather than the many-body wave function as the fundamental variable. Because the density n(r) is a function of only three spatial coordinates, DFT is computationally possible even for enormous systems (rather than the 3 N coordinates of the wave function). The numerical approach, known as the Fast Fourier Transformation, was refined by Cooley and Tukey in 1965, and this had a huge impact on spectral analysis methods. In spectrum analysis, the value of the Fourier process is shown by the power density or power range continuum. The autocorrelation function of a continuous signal also plays a significant role. The Dirichlet condition and zero means for the continuous operation will be provided by the Fourier transform of a finite continuous signal and their relationship to infinite, continuous signals. The compound’s experimental measurements in our paper are just for a short period of time. The record duration can be reduced to a given period T by multiplying the infinite continuous recording by a data window defined.

$$W(\alpha) = \sqrt{\frac{2}{\pi}} \frac{\sin(T\alpha)}{T\alpha}$$  \hspace{1cm} (1)

The window in Fourier integral leads to the identity as.

$$w(t) = 1 \text{ for } |t| \leq \frac{T}{2}$$  \hspace{1cm} (2)

The Fourier transform of this product is the transformation of the infinite record which is paired with transformations of the window when multiplying the infinite record. The Convolution Theorem establishes this relationship, which affirms that:

$$F[f(t) \cdot w(t)] = F(f) \ast W$$  \hspace{1cm} (3)

Discrete-time Fourier transform (DTFT) helps calculate the diffracted wave information and the obtained peaks tell us all about the molecular design’s properties without having to measure the molecular structure. The DTFT is in the direction of x, y, z for a given compound.

$$C = \frac{1}{abc} \int_{0}^{a} \int_{0}^{b} \int_{0}^{c} \rho(x, y, z)e^{-j\left(\frac{2\pi a}{\lambda} x + \frac{2\pi b}{\lambda} y + \frac{2\pi c}{\lambda} z\right)} \, dx \, dy \, dz$$  \hspace{1cm} (4)

The ρ(x, y, z) gives the density distribution of the crystalline state of the compound and (a,b,c) represents the edge length in the (x,y,z) directions. The DTFT biosynthesis analysis of Cu2O as shown (Fig. 1) reveals a distinct difference in the spectral density peak for the three experiments. DTFT peaks shown above indicate that the peak value of 1100 is unique to the synthesized compound and that of the previous compound, the lower peak of 200 is. The sharp rise in maximum value also indicates that the compound is more active and reactive than the other compound.

UV–Vis Analysis

The optical properties of biomolecules loaded Cu2O NPs were analyzed through UV–Vis absorbance spectra. Figure 2 shows the optical absorbance spectra of the Cu2O NPs. The formation of Cu2O NPs confirmed by the color change of copper nitrate aqueous solution from bluish green to sea green when adding Datura metel L. leaf extract shown (Fig. 3). The SPR absorbance peak was found at 790 nm by
the oscillation of electrons on the surface of the Cu$_2$O NPs, which is revealing the reduction of Cu$_2$O NPs. The formed Cu$_2$O NPs absorbance peak at 790 nm shows the electronic d-d transitions made by the Cu$^{2+}$ ions in d orbital, in this kind of absorption favored for the extended lifetime of photogenerated carriers [26]. The serious alkaloids present on the Datura metel L. extract such as hyoscyamine, atropine is exhibited the characteristic absorption band at 200–350 nm in UV–Vis spectra corresponding to π-π* transition [27]. According to Tauc’s plot analysis, the bandgap energy of prepared Cu$_2$O nanoparticles is 2.98 eV. This bandgap energy is ideally suited for solar cell and optical device applications inconsistent with previous research reports suggested by Singh et al. Grad et al. and Kannan et al.

![Figure 1](image1.png)

**Fig. 1** The spectral characterization with a Fourier Transform of the proposed Cu$_2$O compound results. The higher transformation of the high frequency suggests the biosynthesized Cu$_2$O

![Figure 2](image2.png)

**Fig. 2** UV–Vis absorption spectra of Cu$_2$O NPs and bandgap determination also represented in inserted image
Through the annealing method, Grad et al. achieved 2.98 eV for nonlinear optical susceptibility, while Singh et al. achieved the same bandgap energy for nanocrystalline CdTe film for electroluminescent display devices [28, 29].

XRD Analysis

Crystallinity, size, and phase of the biosynthesized Cu₂O NPs were determined through XRD analysis, and their diffraction pattern shown (Fig. 4). Biosynthesized Cu₂O NPs have characteristic diffraction peaks at 2θ angle 22.77°, 25.08°, 26.54°, 29.48°, 31.28°, 32.95°, 36.47°, 38.67°, 42.19°, 47.66°, and 51.62°. The existence of Cu₂O NPs is indicated by the observed diffraction reflections peaks at 29.48°, 36.47°, 42.19°, and 51.62°, which are indexed by Bragg's reflections (110), (111), (200), and (211). According to JCPDS Card No: 77–0199, the specified lattice planes (110), (111), and (200) show primitive Cu₂O NP lattice structures. Other researchers have found similar Cu₂O NPS XRD diffractograms for other plant extracts [6, 12, 31]. The star symbol represents the remaining unassigned peaks and background noises in the XRD pattern, which displays the Datura metel L. proteins enclosed around the Cu₂O NPs [32]. The average crystallite size of the generated Cu₂O NPs is 19.56 nm, as determined by XRD analysis using Debye–Scherer's equation.

\[ D = \frac{k\lambda}{\beta \cos \theta} \]  

In this case, \( k \) is the dimensionless shape factor taken as 0.9, \( \lambda \) known as X-ray wavelength, \( \beta \) is line broadening at half the maximum intensity (FWHM) and \( \theta \) is the Bragg angle. This result illustrated biomolecules are well bound with Cu₂O nanoparticles during synthesis and Datura metel L. extract is one of the promising candidates for reduction and stabilization of Cu₂O NPs.

Fourier Transform Infrared Spectroscopy Analysis

The FTIR spectra analysis revealed the presence of phytochemicals in the plant extract as well as the production of Cu₂O. The IR spectra of Cu₂O NPs are exhibited in comparison to Datura metel L. (Fig. 5). The broad absorption band at 3406 cm⁻¹ in the FTIR spectrum of Datura metel L. leaf extract (Fig. 5b) is attributable to the O–H stretching mode of phenol and alcohols. The peak at 2937 cm⁻¹ indicates C-H stretching of alkyl groups and strong peaks 1651 cm⁻¹ show the C=O stretching vibration of carboxylic groups. The peaks at 1546 cm⁻¹ reveal that the C-N stretch of aliphatic amines and peaks at 1406, 1359, and 1317 cm⁻¹ are representing the C–C stretch (in-ring) of aromatics, N=O bending vibration of nitro compounds, C-N stretch of aromatic amines, respectively. The peaks that appeared at 1105, and 1068 cm⁻¹ are belonging to the C-N stretch of aliphatic amines. The peaks at 752, 621, and 526 cm⁻¹ are shown the existence of C–Cl stretch alkyl halides, C-H bends alkanes, and C-I stretches aliphatic iodo compounds. The FTIR spectrum of Cu₂O NPs showed again the presence
of O–H stretching mode of phenol and alcohols and C-H stretching of alkyl groups at 3404, and 1620 cm\(^{-1}\), which supports the idea of phenol, alcohols, and alkyl group, are free from Cu\(_2\)O NPs formation. The peaks at 1409, 1359, and 1317 cm\(^{-1}\) on Cu\(_2\)O NPs represent a diminishment of C–C stretch (in-ring) of aromatics, N=O bending vibration of nitro compounds, C-N stretch of aromatic amines, respectively. After bioreduction, peak shifts have occurred at 752 to 709 cm\(^{-1}\) on C–Cl alkyl halides, 621 to 650 cm\(^{-1}\) on the C-H bend of alkanes, and 526 to 609 cm\(^{-1}\) on C-I stretch in aliphatic iodo compounds. Above mentioned bio-compounds are acting as a capping agent as well as bound along with the Cu\(_2\)O nanoparticles. The absence of peaks at 2937, 1546, 879 cm\(^{-1}\) and the production of new peaks at 1043, 999 cm\(^{-1}\) reveals that structural changes on NP formation are caused by C–H stretching of alkyl, C-N stretch of aliphatic amines, N–H bending vibration of nitro compounds, and C=O of carboxylic acid. The strong peaks obtained at 819 cm\(^{-1}\) and the existence of new peaks at 499 cm\(^{-1}\) are corresponding to the characteristic formation of Cu\(_2\)O NPs (Fig. 5a) [33]. Particularly aliphatic amines in Datura metel L. leaf extract are mainly responsible for the reduction of copper ions into Cu\(_2\)O NPs. The tentative values of peak assignments are given in Table 1.

### DFT Analysis

A molecule's or crystal's optical qualities are one of the most useful types of parameters for predicting different traits. These can be used to locate wavelengths of optical radiation in the absorption or emission spectrum based on their electronic structure. DFT lets us calculate these properties, related to electron motion evolution under electric field control. DFT is the theory of differential and functional functions. The spectrum data are shown (Fig. 6). NUM is first standardized with [01] which Gaussian has reoriented to speed up the two calculations of electron energy models. Spectral data measurements were used to determine the internal nuclear energy. The Hamiltonian Fock matrix is then used to measure each electron transaction. Once, we know the propagation of the electron, we measure the angular momentum of the electrons that are then used to detect an electron's energy gap.

The energy of the synthesized compound stabilized over some time to a constant value of 16.6378 eV and remained the same indicating compound stability. As seen in Fig. 6, the first fluctuation is caused by the electron's excitation, which eventually returns the electron to its normal state. The oscillation reaction indicates that the compound is irregular, yet the proposed molecule's behaviour is extremely stable.

### Computational Modeling

MERA software was used to calculate the thermodynamic and surface characteristics of Cu\(_2\)O thin films at all temperatures, using periodic boundary conditions and the a, b, and c axes of the Cu\(_2\)O unit cell, as described in [34, 35] and used in studies of organic, inorganic, and combined systems in [34–48].

The MOPS algorithm has been used to model oxyhydrate gel formation [34, 39, 43], crystal structures of trisomium clusters [35, 37, 38, 42, 44, 47, 49, 50], organic molecule

---

Table 1 FTIR wavenumber and their corresponding functional group analysis of Cu\(_2\)O synthesized by Datura metel L

| Wavenumber (cm\(^{-1}\)) | Vibrational assignments | Functional groups |
|--------------------------|------------------------|------------------|
| 3406 | 3404 | O–H stretching | phenol, alcohols |
| 1651 | 1620 | C=C stretching | carboxylic groups |
| 1406 | 1409 | C–C stretch (in-ring) | Aromatics |
| 1359 | 1359 | N=O bending | nitro compounds |
| 1317 | 1317 | C-N stretch | aromatic amines |
| 1105 | 1124 | C-N stretch | aliphatic amines |
| 1068 | 943 | C-N stretch | aliphatic amines |
| 752 | 709 | C-Cl stretch | alkyl halides |
| 621 | 650 | C-H bend | Alkanes |
| 526 | 609 | C-I stretch | aliphatic iodo |
| 2937 | - | C-H stretching | Alkyl |
| 1546 | - | C-N stretch | aliphatic amines |
| 879 | - | N–H bending vibration | nitro compounds |
| - | 819 | Characteristic formation of Cu\(_2\)O NPs | |
| - | 499 | | |
complexation during chemical reactions [45], protein affinity [48], and crystal structures and interaction energies of gas hydrates [40, 51]. Calculated energies, thermodynamic properties (such as enthalpies, entropies, and Gibbs-free energies), modeled structures of complexes, crystals, and clusters, and predicted yields, rates, and regio- and stereospecificity of reactions were all in good agreement with experimental results which previously stated in publications as mentioned above.

DFT B3LYP 6-311G (d,p) level of theory, the structures of hyoscyamine and atropine were optimized. The UV–Vis spectra were then estimated using TD DFT B3LYP 6-311G (d,p), which revealed that the absorption band is 253.3 nm, which matches the experimental data well.

The initial structure for the computer modeling of Cu₂O nanoparticles was cuprite [52] (Crystallography Open Database ID 1000063) (cubic syngony, space group Pn 3 m, a = b = c = 4.252(2), α = β = γ = 90°).

1000 multiplications of the crystal cell in random directions were performed to the composition Cu₂O₂₄₇₄O₁₂₃₇ (this composition corresponds to the experimental size of the particles) and the structure with the minimum energy is chosen. Calculation using the Bragg’s equation showed that the resulting modeled nanoparticles should have diffraction reflections peaks at 20 angle 29.69°, 36.57°, 42.49°, 52.69°, 61.65°, 69.90°, 73.86°, 77.74°, 85.35°. The first four reflections are in good agreement with the experimental diffractogram and correspond to reflections (110), (111), (200), and (211) that show a good quality of the simulation.

The initial structure of atropine and hyoscyamine in an aqueous solution (they are similar since atropine is a racemate and hyoscyamine is an L-isomer of the same compound) modeled within the MOPS software [34, 39, 43] with the continual account of the solvent influence shown (Fig. 7a). The structure contains the intramolecular hydrogen bond = O…H–O with a length of 2.22 Å.

Following that, a model of this nanoparticle’s combination with hyoscyamine and atropine was created. The complex formation’s computed Gibbs free energy is -179.4 kJ/mol. During the formation of the complex, the structure and conformation of atropine (hyoscyamine) are nearly constant. Three short contacts make up the complex (Fig. 7b). Two of them (2.16 Å and 2.19 Å) are carried out by carbonyl oxygen with two copper atoms in nanoparticles. These bifurcate interactions are made possible by a flaw on the nanoparticles’ surface, which occurs when two copper atoms lose their valence at the same time. The third point of contact is the hydroxyl hydrogen of atropine forming a hydrogen bond

Fig. 6 Energy (eV) versus DFT iterations show the compound’s stability after 10 iterations, since the energy levels obtain a constant value and remain the same

Fig. 7 The structure of a) atropine and b) its complex with the fragment of Cu₂O NPs
with the oxygen on the nanoparticle surface (2.09 Å). The intramolecular hydrogen bond = O⋯H–O is preserved, but it is slightly lengthened to 2.37 Å.

Conclusions

A simple and cost-effective technique for the manufacture of Cu2O nanoparticles at room temperature within 30 min has been proposed, with plentiful, underappreciated plant extract (Datura metel L.) being used as a reducing and stabilizing agent. The UV–Vis analysis shows Cu2O NPs formation at 790 nm through the making of Cu2+ ions transition in d-orbital. The result of the XRD pattern reveals that biomolecules of Datura metel L. encapsulation on synthesized Cu2O NPs and found in crystalline nature with an average crystallite size of 19.56 nm. This biomolecules encapsulation is validated by FTIR characterization, the aliphatic amines in Datura metel L. responsible for the reduction of Cu2O NPs, and their Phytochemicals are effectively utilized as a bio-capping agent and it has been bound along around the Cu2O NPs. The energy band stability and spectral fingerprints of the synthesized molecule were investigated using DFT and Fourier power spectrum. We were able to calculate the stability and distinctive spectral signature of the proposed Cu2O compounds using these two computational analyses. For the first time, we successfully used Fourier transform spectral characterization to biosynthesized Cu2O NPs and emphasized their spectrum. The high frequency of spectrum characterization shows that produced Cu2O NPs are more active and reactive than other compounds, yet oscillation reactions are unpredictable, and their behavior is extremely stable even after ten iterations of density functional theory analysis. Furthermore, the current data is being used to research nanoparticles stability in solar cells, wastewater treatment, and biological applications.

Acknowledgements The project was supported by Ministry of Science and Higher Education of Russia (Grant no. FENU-2020-0019). Authors (KC, KG) acknowledged Kalasalingam Academy of Research and Education, Krishnankoil, Tamilnadu, India.

Authors’ Contributions Experimental and characterization of green synthesized Cu2O nanoparticles using Datura Metel L. done by KC and supervised by KG, KK, MGR and RT. Theoretical studies performed by KG, VM, VP and MG and supervised by VP and VM. Manuscript written by KC and checked by all authors.

Funding The project was supported by Ministry of Science and Higher Education of Russia (Grant no. FENU-2020-0019).

Data Availability All data generated during this study are included in this published article.

Declarations

Ethical Approval Not applicable.

Consent to Participate Not applicable.

Consent for Publication Not applicable.

Conflict of Interest The authors declare that they have no known competing financial interests.

References

1. Karthik K, Qadir AM (2019) Synthesis and Crystal Structure of a New Binuclear Copper(II) Carboxylate Complex as a Precursor for Copper(II) Oxide Nanoparticles. J Struct Chem 60:1126–1132. https://doi.org/10.1134/S002247661907014X
2. Kannan K, Radhika D, Vijayalakshmi S, Sadasivuni KK, Ojaiu AA, Verma U (2020) Facile fabrication of CuO nanoparticles via microwave-assisted method: photocatalytic, antimicrobial and anticancer enhancing performance. Int J Environ Anal Chem. https://doi.org/10.1080/03067319.2020.1733543
3. Kannan K, Radhika D, Nikolova MP, Andal V, Sadasivuni KK, Krishna LS (2020) Facile microwave-assisted synthesis of metal oxide CdO-CuO nanocomposite: Photocatalytic and antimicrobial enhancing properties. Optik 218:165112. https://doi.org/10.1016/j.ijleo.2020.165112
4. Azhar W, Khan AR, Muhammad N, Liu B, Song G, Hussain A, Yasin MU, Khan S, Munir R, Gan Y (2020) Ethylene mediates CuO np-induced ultrastructural changes and oxidative stress in arabidopsis thaliana leaves. Environ Sci Nano 7:938–953. https://doi.org/10.1039/C9EN01302D
5. Rajasekar S, Muthuvel A, Kannan K, Chinniaah K, Maik V, Gohulkumar M, Gurushankar K (2021) Synthesis and characterization of undoped and mn-doped copper oxide nanoparticles. Macromol Symp 400:2100122. https://doi.org/10.1002/masy.202100122
6. Jadhav MS, Kulkarni S, Raikar P, Barretto DA, Vootlac SK, Raikar US (2018) Green biosynthesis of CuO & Ag–CuO nanoparticles from malus domestica leaf extract and evaluation of antibacterial, antioxidant and DNA cleavage activities. New J Chem 42:204–213. https://doi.org/10.1039/C7NJ02977B
7. Kargar A, Jing Y, Kim SJ, Riley CT, Pan X, Wang D (2013) ZnO/CuO Heterojunction branched nanowires for photoelectrochemical hydrogen generation. ACS Nano 7(12):11112–11120. https://doi.org/10.1021/nn404838n
8. Wongrakpanich A, Mudunkotuwa IA, Geary SM, Morris AS, Mapuskar KA, Spitz DR, Grassian VH, Salem AK (2016) Size-dependent cytotoxicity of copper oxide nanoparticles in lung epithelial cells. Environ Sci Nano 3:365–374. https://doi.org/10.1039/C5EN00271K
9. Awed AS, El-Ghamaz NA, El-Nahass MM, Zeyada HM (2019) Linear and nonlinear optical properties of alizarin red S thin films. Indian J Phys 93:861–868. https://doi.org/10.1007/s12548-018-01359-6
10. Karthik Kannan D, Radhika DG, Lakkaboyyna SK, Sadasivuni KK, Gurushankar K, Hanafia MM (2021) Photocatalytic and antimicrobial properties of microwave synthesized mixed metal oxide nanocomposite. Inorg Chem Commun 125:108429. https://doi.org/10.1016/j.inoche.2020.108429
11. Gurushankar K, Rimac H, Potemkin V, Grishina M (2021) Investigation of the newly characterized baimantuoluoamide a and baimantuoluoamide b alkaloids as potential cyclin-dependent kinase 4 (CDK4) inhibitors using molecular docking and molecular dynamics simulations. J Mol Struct 1230:129925. https://doi.org/10.1016/j.molstruc.2021.129925

12. Siddiqui VU, Ansari A, Chauhan R, Siddiqui WA (2021) Green synthesis of copper oxide (CuO) nanoparticles by punica granatum peel extract. Materials Today Proceedings 36:751–755. https://doi.org/10.1016/j.matpr.2020.05.504

13. Nasir B, Baig MW, Majid M, Ali SM, Khan MJl, Kazmi STB, Haq I (2020) Preclinical anticancer studies on the ethyl acetate leaf extracts of Datura Stramonium and Datura Inoxia. BMC Complement Med Ther 20:188. https://doi.org/10.1186/s12906-020-02975-8

14. Tian L, Zhou Q, Wang X, Wood TE, Wang L, Duchesne PN, Wu Y, Ouzin GA (2019) Cuprous oxide (Cu2 O) nanoparticles and Cu2 O/N–TiO2 for thin film solar cells applications. Sol Energy Mater Sol Cells 82:315–330. https://doi.org/10.1016/j.solmat.2004.02.006

15. Siddiqui VU, Ansari A, Chauhan R, Siddiqui WA (2021) Green synthesis of copper oxide (CuO) nanoparticles by punica granatum peel extract. Materials Today Proceedings 36:751–755. https://doi.org/10.1016/j.matpr.2020.05.504

16. Muthukrishnaraj A, Al-Zahrawi SA, Al Otaibi A, Kalavassi SS, Manikanand A, Balasubramanian N, Bilgrami AL, Ahamed MAR, Khan A, Asiri AM, Balasubramanian N (2021) Enhanced photocatalytic activity of Cu2 O Cabbage/RGO nanocomposites under visible light irradiation. Polymers 13:1712. https://doi.org/10.3390/polym13111712

17. Koiki BA, Arotibah OA (2020) CuO as an emerging semiconductor in photocatalytic and photoelectrochemical treatment of water contaminated with organic substances: a review. RSC Adv 10:36514–36525. https://doi.org/10.1039/D0RA06585F

18. Ramesh C, Hariprasad M, Ragunathan V (2011) Effect of Arachis hypogaea L. leaf extract on Barfoed’s Solution; Green synthesis of CuO nanoparticle and its antibacterial effect. Curr Nanosci 7:995–999. https://doi.org/10.2174/1573413117982020781

19. Aboud Y, Safaj T, Chagraoui A, Bouari AE, Brouki K, Tanane O, Ilhssane B (2014) Biosynthesis, characterization and antimicrobial activity of copper oxide nanoparticles (CuONPs) produced using brown alga extract (Bifurcaria bifurcata). Appl Nanosci 4:571–576. https://doi.org/10.1007/s13204-013-0233-x

20. Kerour A, Boudjadar S, Bourrazi R, Allouche B (2018) Eco-friendly synthesis of cuprous oxide (Cu2O) nanoparticles and improvement of their solar photocatalytic activities. J Solid State Chem 263:79–83. https://doi.org/10.1016/j.jssc.2018.04.010

21. Haunsch R, Barth A, French BA (2019) Comprehensive analysis of the history of DFT based on the bibliometric method RPS. J Chiminform 11:72. https://doi.org/10.1186/s13321-019-0395-y

22. Ferri E (1928) Eine Statistische Methode Zur Bestimmung Einiger Eigenschaften Des Atoms und ihre Anwendung auf die Theorie des periodischen Systems der Elemente. Z Physik 48:73–79. https://doi.org/10.1007/BF01351576

23. Haunsch R, Barth A, Marx W (2016) Evolution of DFT studies in view of a scientometric perspective. J Chiminform 8:52. https://doi.org/10.1186/s13321-016-0166-y

24. Ciacci EJ, Biviano AB, Whang W, Coromilas J, Garan H (2011) A new transform for the analysis of complex fractionated atrial electrograms. BioMed Eng OnLine 10:35. https://doi.org/10.1186/1475-925X-10-35

25. Mesgaran SD, Eggert A, Höckels P, Derno M, Kuhla B (2020) The use of milk Fourier transform mid-infrared spectra and milk yield to estimate heat production as a measure of efficiency of dairy cows. J Animal Sci Biotechnol 11:43. https://doi.org/10.1186/s40104-020-00455-0

26. Luo Z, Jiang H, Li D, Hu L, Geng W, Wei P, Ouyang P (2014) Improved photocatalytic activity and mechanism of Cu2O/N–TiO2 prepared by a two-step method. RSC Adv 4:17797–1804. https://doi.org/10.1039/C4RA47973K

27. Ramalechume C, Shamili P, Krishnaveni R, Swamidoss CMA (2020) Synthesis of copper oxide nanoparticles using tree gum extract, its spectral characterization, and a study of its antibacterial properties. Materials Today Proceedings 33:4151–4155. https://doi.org/10.1016/j.matpr.2020.06.587

28. Singh RS, Kangari VK, Sanagappalli S, Jayaraman V, Mahendra S, Singh VP (2004) Nano-structured CdTe, CdS and TiO2, for thin film solar cell applications. Sol Energy Mater Sol Cells 82:315–330. https://doi.org/10.1016/j.solmat.2004.02.006

29. Grad L, Novotny Z, Hengsberger M, Osterwalder J (2020) Influence of surface defect density on the ultrafast hot carrier relaxation and transport in Cu2O photoelectrodes. Sci Rep 10:10686. https://doi.org/10.1038/s41598-020-67589-z

30. Kannan K, Radhika D, Gnanasangeetha D, Krishna LS, Gurushankar K (2021) Y3+ and Sm3+ co-doped mixed metal oxide nanocomposite: Structural, electrochemical, photocatalytic, and antibacterial properties. Applied Surface Science Advances 4:100085. https://doi.org/10.1016/j.aspadv.2021.100085

31. Sasidharan D, Namitha TR, Johnson SP, Jose V, Mathew P (2020) Synthesis of silver and copper oxide nanoparticles using myristica fragrans fruit extract: antimicrobial and catalytic applications. Sustain Chem Pharm 16:100255. https://doi.org/10.1016/j.scpc.2020.100255

32. Sarkar J, Chakraborty N, Chatterjee A, Bhattacharjee A, Dasgupta D, Acharya K (2020) Green synthesized copper oxide nanoparticles ameliorate defense and antioxidant enzymes in lens culinaris. Nanomaterials 10:312. https://doi.org/10.3390/nano10020312

33. Anand GT, Sundaram SJ, Kanimozhi K, Nithiyavathi R, Kaviyarasu K (2021) Microwave assisted green synthesis of CuO nanoparticles for environmental applications. Materials Today Proceedings 36:427–434. https://doi.org/10.1016/j.matpr.2020.04.881

34. Sukharev YI, Potemkin VA, Markov BA (2001) Autowave processes of forming gels as a cause of the coloring of oxhydrate gels (the chromatic effect) of some rare earth metals (yttrium, gadolinium). Colloids Surf A 194:75–84. https://doi.org/10.1016/S0927-7757(01)00757-9

35. Potemkin VA, Maksakov VA, Kirin VP (2003) Conformational states of triosmium clusters with aminoacid ligands: a theoretical study. J Struct Chem 44:741–747. https://doi.org/10.1023/B:JORY.0000029809.88411.8b

36. Potemkin VA, Krasnov VP, Levin GL, Bartashevich EV, Andreeva IN, Kuzminsky MB, Anikin NA, Charushin VN, Chupakhin ON (2004) Kinetic resolution of (±)-2,3-dihydro-3-methyl-4H-1,4-benzoxazine in the reaction with (S)-naproxen chloride: a theoretical study. Mendeleev Commun 14:69–70. https://doi.org/10.1070/MC2004v014n02ABEH010887

37. Potemkin VA, Maksakov VA, Kirin VP (2004) Theoretical study of the conformations of triosmium clusters with a chiral carane ligand. J Struct Chem 45:405–409. https://doi.org/10.1007/s10947-005-0006-9

38. Potemkin VA, Maksakov VA, Korenev VS (2005) Theoretical study of the conformational states of triosmium clusters with a chiral pinane ligand. J Struct Chem 46:43–48. https://doi.org/10.1007/s10947-006-0007-3

39. Sukharev YI, Avidin VV, Lymar AA, Belkanova MY, Potemkin VA (2006) Directions in structure formation of oxhydrate gels of zirconium and rare earth elements. J Struct Chem 47:151–155. https://doi.org/10.1007/s10947-006-0280-1

40. Aladko EY, Ancharov AI, Goryainov SV, Kurnosov AV, Larionov EG, Likhacheva YA, Manakov AY, Potemkin VA, Sheromov MA, Teplykh AE, Voronin VI, Zhurko FV (2006) New type of phase transformation in gas hydrate forming system at high pressures.
Some experimental and computational investigations of clathrate hydrates formed in the SF6–H2O system. J Phys Chem B 110:21371–21376. https://doi.org/10.1021/jp061698r
41. Grishina MA, Potemkin VA, Bartashevich EV, Sinyaev AN, Rusinov GL, Latosh NI, Ganebnykh IN, Koryakova OV, Ishmetova RI (2006) Modeling of 1,2,4,5-tetrazine complexes with organic amines. J Struct Chem 47:1155–1160. https://doi.org/10.1007/s10947-006-0438-x
42. Potemkin VA, Maksakov VA, Korenev VS (2007) Theoretical study of the conformational states of trisium clusters with a chiral μ-1-NH pinane ligand. J Struct Chem 48:225–230. https://doi.org/10.1007/s10947-007-0036-6
43. Avidin VV, Lymar AA, Batist AV, Nikitin EA, Belkanova MY, Potemkin VA (2007) Structure formation in heavy metal oxyhydrates at low rates of gel formation. J Struct Chem 48:747–752. https://doi.org/10.1007/s10947-007-0114-9
44. Korenev VS, Kirin VP, Maksakov VA, Virovets AV, Tkachev SV, Potemkin VA, Agafontsev AM, Tkachev AV (2007) Triosmium cluster with the bridging aminooxime derivative of pinane: synthesis, crystal structure and conformational analysis. Russ J Coord Chem 33:594–600. https://doi.org/10.1134/S1070328407080088
45. Shchur IV, Khudina OG, Burgart YV, Saloutin VI, Grishina MA, Potemkin VA (2007) Synthesis, structure, and complexing ability of fluoroalkyl-containing 2,2′-(biphenyl-4,4′-dilyldihydrazone)-bis(1,3-dicarbonyl) compounds. Russ J Org Chem 43:1781–1787. https://doi.org/10.1134/S107042800712007X
46. Grishina MA, Potemkin VA, Matern AI (2008) Theoretical study of acridane oxidation reactions. J Struct Chem 49:7–12. https://doi.org/10.1007/s10947-008-0002-y
47. Maksakov VA, Pervukhina NV, Podberezhskaya NV, Afonin MY, Potemkin VA, Kirin VP (2008) X-ray and conformation analysis of the new trinuclear cluster of osmium Os3(μ, η2-OCC6H5) (CO)9. J Struct Chem 49:894–900. https://doi.org/10.1007/s10947-008-0002-y
48. Kuzmicheva GA, Jayanna PK, Eroshkin AM, Grishina MA, Pereyaslavskaya ES, Potemkin VA, Petrenko VA (2009) Mutations in Fd phage major coat protein modulate affinity of the displayed peptide. Protein Eng. Des Sel 22:631–639. https://doi.org/10.1093/protein/gzp043
49. Potemkin VA, Ivshina NN, Maksakov VA (2009) Theoretical Study of the conformational features of triosmium clusters. J Struct Chem 50:143–151. https://doi.org/10.1007/s10947-009-0202-0
50. Ivshina NN, Bartashevich EV, Potemkin VA, Grishina MA, Ishmetova RI, Rusinov GL, Latosh NI, Slepukhin PA, Charushin VN (2010) Changes in the vibrational characteristics of substituted 1,2,4,5-tetrazines after complexation with 1,2,3-benzotriazole: A theoretical study. J Struct Chem 50:1053–1058. https://doi.org/10.1007/s10947-009-0155-3
51. Manakov AY, Likhacheva AY, Potemkin VA, Ogienko AG, Kurnosov AV, Ancharov AI (2011) Compressibility of gas hydrates. ChemPhysChem 12:2476–2484. https://doi.org/10.1002/cphc.201100126
52. Neuburger MC (1931) Präzisionsmessung der Gitterkonstante von Cuprooxyd Cu2O. Z Phys 67:845–850. https://doi.org/10.1007/BF01390765

Publisher’s Note Springer Nature remains neutral with regard to jurisdictional claims in published maps and institutional affiliations.