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RESEARCH ARTICLE

Theoretical Study of a Coumarin-Based Colorimetric Sensor for Cu^{2+} Detection Using DFT Calculation

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ABSTRACT

The development of chemosensors for the detection of metal ions that are environmentally and biologically significant remains an important research goal. Herein, we present the rational design of a novel coumarin derivative, *(E)-6-((1H-pyrrol-2-yl)diazenyl)-7-hydroxy-2H-chromen-2-one* (CTD), as a potential colorimetric chemosensor for Cu^{2+} ions. Theoretical studies were conducted using DFT and TD-DFT methods to elucidate the electronic and optical properties of the 1:1 stoichiometric complex molecule formed between CTD and Cu^{2+}. Ground-state geometry optimizations performed with the PBEPBE function and the LANL2DZ basis set revealed that CTD is an effective chelating agent for Cu^{2+}. The absorption maximum of CTD was 410.81 nm as a result of TD-DFT calculations. Following complexation with Cu^{2+}, a significant bathochromic shift of approximately 90 nm was observed, and the absorption of the CTD-Cu^{2+} complex was calculated to be 502.10 nm. This pronounced red shift is indicative of a visible colorimetric response. To reveal the electronic origin of this spectral modulation, a Frontier Molecular Orbital (FMO) analysis was performed. The calculations showed a decrease in the HOMO-LUMO energy gap (E_{gap}) from 1.78 eV for the free CTD molecule to 1.54 eV for the CTD-Cu^{2+} complex. These theoretical findings strongly suggest that CTD is a highly promising candidate for experimental validation as a new generation, visually detectable colorimetric chemosensor for Cu^{2+}.

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1. Introduction

Copper (Cu^{2+}) ion is one of the essential metal ions found in the human body and plays important role in many metabolic and enzymatic processes in living organisms (Fu et al., 2017; Savran et al., 2020; Yang et al., 2023). However, excessive Cu^{2+} acts as a contributing factor in the development of many neurodegenerative disorders, including Amyotrophic Lateral Sclerosis (ALS), Alzheimer's, Parkinson's and Wilson's disease (Ban et al., 2024; Y. Wang et al., 2025; Zhong et al., 2024). While Cu^{2+} is an essential nutrient when ingested in low concentrations, it can be toxic when consumed in excess (Charkiewicz, 2024; Taylor et al., 2020). For these reasons, developing robust, reliable and easy methods for detecting Cu^{2+} ions in environmental and biological settings is extremely

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important. Traditional analytical techniques such as Inductively Coupled Plasma Mass Spectrometry (ICP-MS), Atomic Absorption Spectrometry (AAS) and Atomic Emission Spectrometry (AES), despite offering high sensitivity and accuracy are limited by their low practical applicability, the laboriousness of sample preparation processes and the inability to perform real-time analysis in the field (Heydari et al., 2025; Savran et al., 2020). In this context, colorimetric or fluorimetric optical chemosensors have emerged as powerful and attractive alternatives. Optical chemosensors offer significant advantages due to their high sensitivity and selectivity, ease of use, low cost, and potential for visual detection (Alguno et al., 2025; Yan et al., 2021; Zhang et al., 2022).

The rational design of an effective optical chemosensor molecule generally consists of a signal unit (fluorophore or chromophore) and a recognition unit. Due to their high photophysical properties, coumarin and its derivatives are widely used in chemosensor designs (Karuk Elmas et al., 2022; Polashi et al., 2025; Sarmah et al., 2022).

Density Functional Theory (DFT) and time-dependent DFT (TD-DFT) have become indispensable tools in modern chemosensor development (Guan et al., 2025; X.-F. Sun et al., 2016). These methods enable the prediction of molecular structures, electronic properties and spectroscopic responses in a computational environment, providing a deep insight into the underlying sensing mechanisms (Chen et al., 2017; Udhayakumari et al., 2025). This predictive power not only accelerates the design-synthesis-testing cycle but also guides the development of more efficient and selective sensors by facilitating a deeper understanding of structure-property relationships.

In this study, a new coumarin derivative chemosensor molecule named *(E)-6-((1H-pyrrol-2-yl)diazenyl)-7-hydroxy-2H-chromen-2-one* (CTD) was designed and its binding mechanism and optical response to Cu^{2+} ions were theoretically investigated using DFT and TD-DFT methods. The calculations showed that the bathochromic shift in the absorption spectrum and the decrease in the energy gap between the frontier molecular orbitals upon CTD binding to Cu^{2+} ions that the molecule could function as a potent colorimetric chemosensor.

2. Calculation Methods

All calculations were performed using the Gaussian 09W software package with density functional theory (DFT) and time-dependent DFT (TD-DFT) methods. The Perdew-Burke-Ernzerhof (PBEPBE) approximation and LANL2DZ basis set was used for all atoms, including the Cu^{2+} ion. LANL2DZ basis set provides a consistent theoretical level, particularly suitable for the copper atom, and keeps the computational cost at a reasonable level; this is appropriate for this study, which is conducted for the purpose of preliminary screening and determination of fundamental electronic properties (HOMO-LUMO, UV-Vis transitions). However, it should be noted that LANL2DZ provides a more limited basis set for light elements (C, H, N, O) in terms of polarization and scattering functions and therefore does not yield results as precise as larger basis sets for fine structural details such as bond lengths and vibrational frequencies. Furthermore, since the study was focused on understanding the mechanism of the fundamental interaction between CTD and the Cu^{2+} ion, as well as the resulting changes in the electronic/optical properties, the calculations were performed in an inert environment without the use of any solvent model. This inert environment allowed for the isolation of the behavior of the molecular system in its pure form (Dennington et al., 2009; Frisch et al., 2009; Karagoz et al., 2025; Perdew et al., 1996; J. P. Wang et al., 2012).

The proposed sensor CTD and CTD-Cu^{2+} complex molecules were optimized without applying any symmetry constraints. UV-Vis absorption spectra for the optimized structures were calculated using the TD-DFT method. The first 20 excited states were calculated to adequately cover the relevant spectral region. The calculated excitation energies and oscillator strengths were used to plot the simulated absorption spectra.

Frontier molecular orbitals (FMO), particularly the highest occupied molecular orbital (HOMO) and the lowest unoccupied molecular orbital (LUMO) were visualized for the CTD and the CTD-Cu^{2+} complex. The HOMO-LUMO energy gap was calculated to understand the electronic transitions causing the observed spectral shifts.

3. Results and Discussion

This study thoroughly investigates the colorimetric detection behavior of the newly designed *(E)-6-((1H-pyrrol-2-yl)diazenyl)-7-hydroxy-2H-chromen-2-one* (CTD) molecule toward Cu^{2+} ions at the theoretical level using DFT and TD-DFT methods. The findings revealed the potential of the CTD molecule to detect Cu^{2+} ions colorimetrically at both the structural and electronic levels. The CTD molecule was designed to contain specific binding regions expected to coordinate with Cu^{2+} ions. The geometries of the complex formed by CTD and Cu^{2+} were fully optimized using the DFT/PBEPBE functional with the LANL2DZ basis set (Figure 1). The optimized CTD molecule exhibited a stabilized planar conformation. The calculation results showed that the CTD molecule formed a stable complex with the Cu^{2+} ion in a 1:1 stoichiometry. The Cu-O and Cu-N bond lengths (1.91-1.95 Å) confirmed the strong metal-ligand interaction and the high stability of the complex.

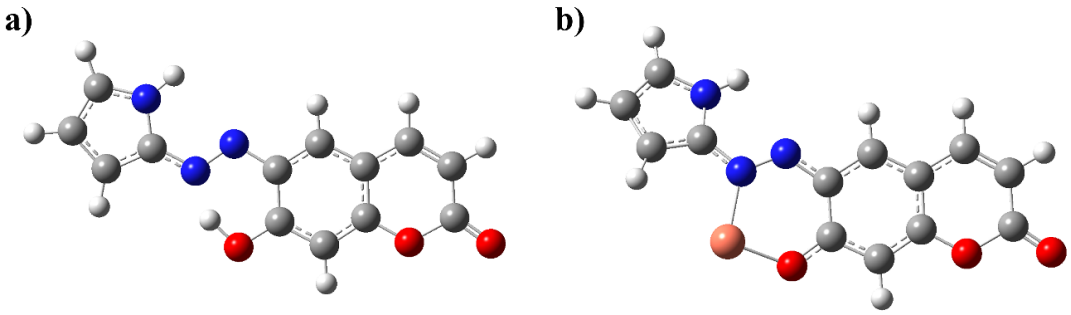

Figure 1. (a) Optimized geometries of CTD and (b) CTD-Cu^{2+} complex (1:1 stoichiometry) calculated at the PBEPBE/LANL2DZ level. Atomic colors: dark gray (carbon), light gray (hydrogen), blue (nitrogen), red (oxygen), orange (copper).

The optical properties of the CTD molecule was investigated using TD-DFT calculations. The simulated UV-Vis spectra for the CTD molecule and the CTD-Cu^{2+} complex were summarized in the Table 1 and shown in the Figure 2. The CTD molecule and the CTD-Cu^{2+} complex showed maximum absorption at 410.81 nm and 502.10 nm, respectively. This significant bathochromic shift of 91.29 nm, which occurs with complex formation, is a theoretical indication of a response that can be easily seen with the naked eye, shifting from violet to green.

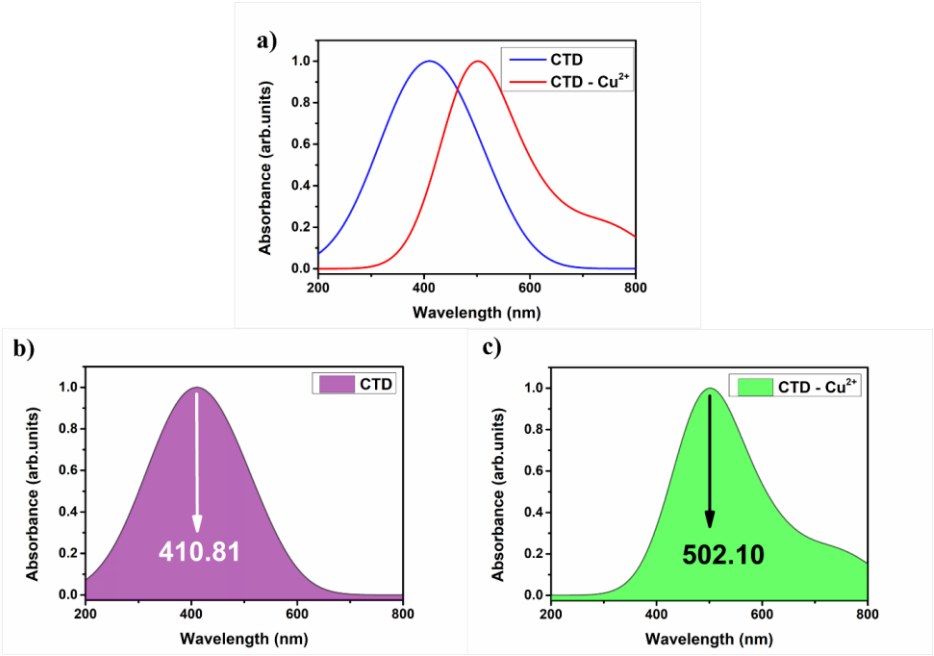

Figure 2. Theoretical absorption spectra of a) CTD and CTD-Cu^{2+} molecules b) CTD molecule c) CTD-Cu^{2+} complex obtained at the PBEPBE/LANL2DZ level using the TD-DFT method.

Table 1. Some electronic properties of CTD and the CTD-Cu^{2+} complex.

	CTD	**CTD - Cu^{2+}**
HOMO (eV)	-5.44	-9.00
LUMO (eV)	-3.66	-7.46
ΔE (eV)	1.78	1.54
TD-DFT Abs. Wavelength (nm)	410.81	502.10

To focus on the electronic cause of the observed spectral changes, the limiting molecular orbitals (HOMO and LUMO) of CTD and the CTD-Cu^{2+} complex were analyzed (Table 1). The basis of the sensing mechanism is based on the decrease in the HOMO-LUMO energy gap (ΔE) resulting from the coordination of CTD with Cu^{2+}. According to calculations, while the ΔE value of CTD was 1.78 eV, it decreased to 1.54 eV in the CTD-Cu^{2+} complex (Figure 3). Considering the proportionality between the absorption energy and the ΔE, this decrease in the ΔE explains the 91.29 nm bathochromic shift.

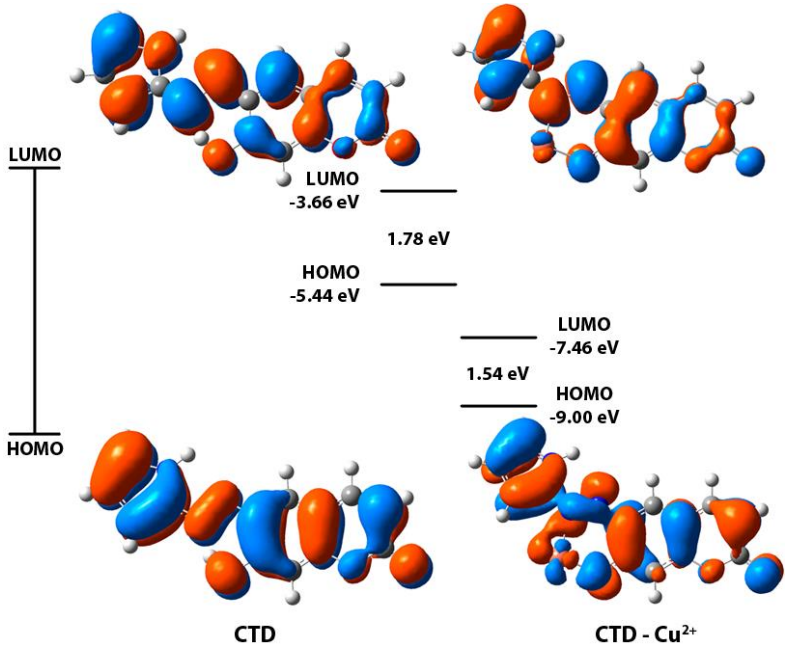

Figure 3. Schematic representation of HOMO and LUMO levels of the CTD molecule and CTD-Cu^{2+} complex calculated at the PBEPBE/LANL2DZ level.

Based on structural, spectral and electronic analyses, the sensing mechanism proceeded via Cu^{2+} coordination in the coumarin oxygen and diazenyl nitrogen regions. This interaction promoted electron transfer from the ligand π system to the Cu^{2+} ion, causing a spectral shift toward red and a visible color change. The 91.29 nm bathochromic shift in absorption demonstrated a visually detectable colorimetric response potential.

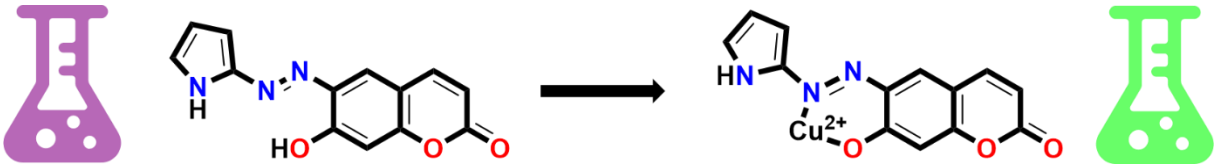

Figure 4. CTD-Cu^{2+} complex formation mechanism.

The predicted bathochromic shift of 91.29 nm, alongside the associated significant color change, is considered to reveal the potential of the designed CTD chemoprobe as a "naked-eye" Cu^{2+} sensor. This finding is held to be consistent with the performance of coumarin-based colorimetric sensors reported in the literature. When some studies on this subject were examined, it was seen that Q. Sun et al. (2026) observed a redshift of 81 nm (from 420 nm to 501 nm), Soufeena et al. (2019) reported a redshift of 82 nm (from 354 nm to 436 nm), and Bhorge et al. (2015) detected a redshift of 85 nm (from 355 nm to 440 nm) by adding Cu^{2+} to the probe. The 91.29 nm bathochromic shift obtained in the present study was demonstrated to exhibited a high degree of concordance, both qualitatively and quantitatively, with the spectral characteristics reported across the literature.

HOMO-LUMO energy gap is utilized as a crucial theoretical indicator of the electronic structural changes occurring upon coordination. This reduction directly is linked to the bathochromic shift observed in the TD-DFT spectra, suggesting an easier electronic transition in the complex (CTD-Cu^{2+}). The calculated HOMO-LUMO energy gap values for the ligand (CTD) and the complex (CTD-Cu^{2+}) were determined as 1.78 eV and 1.54 eV, respectively. This energy decrease (0.24 eV) is deemed consistent with similar studies reported in the literature that investigate ligand-metal interactions. For instance, a decrease in the energy gap from 3.325 eV (ligand) to 2.756 eV (complex) was documented by Niranjan et al. (2025). Furthermore, an even more pronounced reduction was reported by Isaad and El Achari (2022), where the HOMO-LUMO gap was found to decrease from 1.3388 eV for the ligand to 0.2258 eV for the coordinated complex. The magnitude of the energy decrease obtained in the present study was established to support the theoretical framework that the coordination of Cu^{2+} stabilizes the frontier molecular orbitals, thus facilitating the HOMO to LUMO transition and providing the theoretical basis for the observed color change.

Consequently, the PBEPBE/LANL2DZ methodology was confirmed as a reliable tool for predicting the optical properties

and sensing capabilities of colorimetric chemoprobes. The findings obtained in the current study were demonstrated to establish CTD as a promising candidate for a colorimetric Cu^{2+} sensor, with high concordance observed with both theoretical and experimental data available in the literature.

4. Conclusion

In this study, a *(E)-6-((1H-pyrrol-2-yl)diazenyl)-7-hydroxy-2H-chromen-2-one* (CTD) molecule was designed and its potential as a colorimetric chemosensor for Cu^{2+} ions was investigated using DFT and TD-DFT methods. The CTD molecule formed a stable 1:1 stoichiometric complex with the Cu^{2+} ion via the oxygen of the hydroxyl group at position 7 of the coumarin and the nitrogen of the diazenyl group on the pyrole ring. TD-DFT calculations showed that the absorption of CTD shifted from 410.81 nm to 502.10 nm (~91 nm), indicating a visually detectable colorimetric response. Analysis of the frontier molecular orbitals revealed that the HOMO-LUMO energy gap decreased as a result of complexation.

All these theoretical findings indicated that the designed CTD molecule was a promising colorimetric chemosensor candidate, offering the possibility of detecting Cu^{2+} ions by visual observation without requiring additional equipment. This work provided a theoretical foundation for experimental research and encouraged the synthesis of the designed molecule for experimental sensor studies, while also demonstrating the power of computational chemistry in the design of advanced chemical sensor molecules.

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Conflict of Interest

The authors declare that they have no conflict of interest.

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