JURNAL KIMIA VALENSI
p-ISSN: 2460-6065; e-ISSN: 2548-3013
Journal homepage: https://journal.uinjkt.ac.id/index.php/valensi
Research Article

Synthesis and Characterization of Optical Properties of Carbon Quantum Dots (CQD) Based on Mustard Green (*Brassica juncea L*) Leaf with Urea Addition

Elvan Yuniarti[1] and Ai Nurlaela

[1]*Physics Department, Faculty of Science and Technology, UIN Syarif Hidayatullah, Jakarta (15412), Indonesian*
[2]*Education Physics Department, Faculty of Education, UIN Syarif Hidayatullah (15412), Indonesian*

Email: elvan.yuniarti@uinjkt.ac.id

Article Info
Received: Aug 3, 2023
Revised: Sept 13, 2023
Accepted: Nov 21, 2023
Online: Nov 15, 2023

Citation:
Yuniarti, E., & Nurlaela, A. (2023). Synthesis and Characterization of Optical Properties of Carbon Quantum Dots (CQD) Based on Mustard Green (Brassica juncea L) Leaf with Urea Addition. *Jurnal Kimia Valensi*, *9*(2), 253-260

Doi: 10.15408/jkv.v9i2.34164

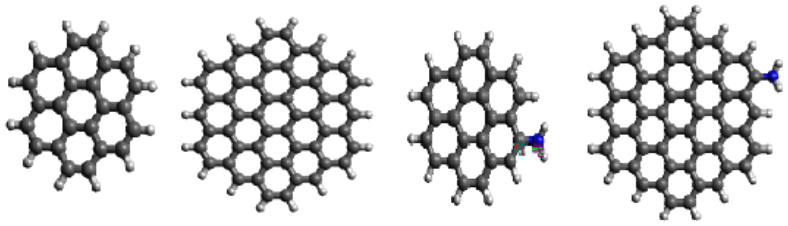
Abstract
Carbon quantum dots (CQDs) are a class of fluorescent carbon nanomaterials. Carbon quantum dots (CQDs) were synthesized in this work from Mustard Leaves (*Brassica juncea* L) with the Addition of Urea via a microwave-assisted reflux method. This research aims to characterize CQDs' optical properties, energy gap, and emission under UV light computationally and experimentally. The studied optical properties obtained the maximum absorption peak observed from the UV-Vis spectrum of CQDs without urea shown at 233 nm. The UV-Vis spectrum of CQDs with the addition of urea (1 g, 1.5 g, and 2 g urea) has maximum absorption peaks at 424 nm, 422 nm, and 418 nm. The addition of urea causes a shift in the peak of the UV-Vis absorption spectrum towards red wavelengths (redshift). CQDs display bright green emissions when exposed to UV irradiation. In this work, the structures of CQDs of various forms (CQD-24, CQD-54, CQD-24-NH_2, CQD-54-NH_2) are theoretically studied in detail, and the results present both models (CQD-24, CQD-54) shows that the calculation results are in accordance with the experimental results, namely having a maximum UV-Vis absorption at 233 nm and in the range 200-400 nm. The results of calculations based on experiments show the same trend, namely that with the addition of urea, there is a shift in the absorption peak (redshift). The gap energy obtained also decreased with the addition of urea. CQDs solution emits yellow-green light.

Keywords: CQD, DFT, gap energy, TDDFT, UV-Vis

1. INTRODUCTION

Carbon Quantum Dots (CQD) is a glowing nanomaterial that attracts the attention of some researchers; CQD has a size of about 10 Nm. CQD has low toxicity properties and strong photoluminescence, and biocompatibility is excellent, highly tunable photoluminescence behavior [1]. In addition, CQD can be easily synthesized from natural materials with simple techniques. Therefore, CQD can be fabricated on a large scale. Various applications of CQD materials have been utilized as solar cells [2], displays, cancer detection, drug delivery carriers in biomedicine, absorbing material in photovoltaics [3], biomedical, fluorescent detection of Escherichia coli [4], and gas sensor [5].

The abundant raw material has led to much research on CQD from natural ingredients derived from plant parts such as fenugreek seeds [6], watermelon rinds [7], cucumber and green pepper [8], Catharanthus roseus (white flowering plant) leaves [9], milk, pepper, coriander, honey, garlic, curcumin, rice husks [10]. Apart from that, it has been synthesized from green mustard stems, green mustard leaves, Cerbera manghas skin, Cerbera manghas flesh, yellow pumpkin skin, and yellow pumpkin flesh [11]. From these studies, it was reported that the obtained CQD have good optical properties such as improved visible-light absorption (320-650 nm), high fluorescence (720-840nm). Previous research also observed the gap energy of CQDs originating from natural materials, namely from 1.9 eV to 3.0 eV[11]. Therefore, CQD can be used as dyes in quantum dot-sensitized solar cells (QDSSC) [12]. This is consistent with the optical properties of CQD, which can absorb the spectrum



(a) (b) (c) (d)

Figure 1. The CQD structure before optimization (a.) CQD-24, (b.) CQD-54 (c.) CQD-24-NH_2 (d.) CQD-54-NH_2

of sunlight. The results of other studies also reported the photoluminescent optical properties of CQD, which can transmit a spectrum of light strongly, so that CQD has the opportunity to be used in the medical field as bioimaging or in the light-emitting (LED) [13].

Computational CQD research has been widely carried out. CQD can be modeled as a graphene quantum dot shape. This research used computational analysis and interaction experiments of CQD with phenol in river water [14]. Carbon nanoparticles that have less than 10 nm in size are called Cdots. CQD can also be modeled as Cdot [15]. Many computational studies use Density Function Theory (DFT) and Time-Dependent Density Functional Theory (TD-DFT) methods. The DFT method has several advantages, including an efficient approach to calculating electronic properties, the ability to calculate complex organic molecules or solid materials, more computational precision with the GGA (Generalized Gradient Approximation) approach and more precise Meta GGA calculations [16]. Another method used is TD-DFT, which can predict absorption spectra regarding electronic properties in chemical processes [17]. In this study, the calculations were carried out using the DFT and TD DFT. Calculations were performed to determine the electronic and optical properties of the CQDs. other studies have calculated the electronic and optical properties for N, P-doped CQDs [18].

This research aims to synthesize CQDs based on Mustard green (*Brassica juncea* L) leaf with Urea addition and characterize the optical properties of CQDs (maximum absorption and light emission of CQDs solutions). Apart from that, this research also calculated the energy gap of CQDs experimentally and computationally.

2. RESEARCH METHODS

Experiment Method

Preparation of Materials for Making CQD

The synthesis of Carbon Quantum Dots (CQD) begins by preparing the ingredients: mustard leaves (20 g), urea (1, 1.5, and 2 g), and distilled water (140 ml). Mustard leaf extract is obtained by mixing 20 g of mustard leaves with 140 ml of distilled water in a household blender. After mixing thoroughly, the solution is filtered using Whatman 40 filter paper to separate the part of the sample that is still coarse from the desired solution. 20 ml of the filtered solution from the previous stage was taken into the crucible. After that, the urea was weighed with varying masses of 1 g, 1.5 g, and 2 g to be mixed with the mustard leaf solution. Next, the mustard leaf and urea solution were made into carbon dots using the green synthesis method by heating with a microwave for 15 minutes [19]. The solution will turn into a brownish crust that sticks to the bottom of the container. This color indicates that CQD has been formed. Then, the precipitate was separated by drying at 60^{o}C for one hour. Then, add 10 ml of distilled water and centrifuge, then pour in the carbon dots obtained by heating them on a hot plate. In order to obtain different samples, repetitions were carried out with the addition of different urea concentrations. Next, the optical properties of the CQDs were characterized by UV–Vis spectrophotometer. The CQD characterization results were analyzed for their optical properties, calculate and analyzed the gap energy using the touch plot method [20].

Computational Method

CQD has been modeled **(Figure 1)** by reducing graphene to CQD-24 carbon atoms and CQD-54 carbon atoms. Another model was by adding an NH_2 functional group. Then, the model was optimized with the DFT method and calculated the optical properties with the TDDFT method. Calculations were performed using Orca 5.0 software [21].

3. RESULTS AND DISCUSSION

The UV-Vis CQD absorption spectra pattern of mustard leaf extract without adding urea, the addition of 1 g, 1.5 g, and 2 g urea, is shown in Figure 2. A red line spectrum shows the UV-Vis CQD absorption spectrum pattern without adding urea. The UV-Vis absorption spectrum of CQD without adding urea is in the absorption range of

200-400 nm and has maximum absorption intensity at a wavelength of 233 nm. This spectrum shows that 233 nm was assigned to the typical $\pi \rightarrow \pi^*$ transition of the conjugated C=C bond [22]. The green line spectrum in **Figure 2** represents the CQD resulting from adding 1 g of urea. This UV-Vis absorption spectrum has an absorption wavelength of 300 nm to 500 nm and has a maximum absorption intensity at a wavelength of 424 nm. It shows n–π^* transition C=O [23] [24]. The UV-Vis absorption spectrum pattern of CQD mustard greens with adding 1.5 g of urea can be seen in the blue line spectrum (**Figure 2**). This spectrum has an absorption range of 300-500 nm and has a maximum absorption at a wavelength of 422 nm. The UV-Vis spectrum pattern of CQD produced by adding 2 g of urea to mustard leaf extract is shown by the spectrum of the yellow line in **Figure 2**. This spectrum has a 300-500 nm range with an absorption peak of 418 nm. The addition of urea causes a shift in the peak of the UV-Vis absorption spectrum towards the red wavelength (red shift). Urea contains carbon, oxygen, nitrogen, and hydrogen [25]. Functional groups of NH_2 can interact with the surface of CQDs. NH_2 from urea acts as an electron donor, causing redistribution of electrons in CQD and giving rise to a new state in the gap energy, which produces new HOMO-LUMO, which produces a lower gap energy (redshift) [26].

Based on the TD-DFT calculation, the UV-Vis spectra results agree with the experiment's (**Figure 3**). The calculation results for CQD- 24 (**Figure 3a**) have an absorption opportunity in the wavelength range of 150-240 nm and 250-300 nm. Calculations to model the larger CQD are carried out by increasing the number of carbon atoms to 54 carbon atoms (CQD-54). CQD-54 (**Figure 3c**) has an absorption opportunity at wavelengths of 250-300 nm and 350-400 nm. The two models show that the calculation results are under the experimental results, which have a maximum absorption at 233 nm and are in the 200-400 nm range.

The addition of urea is modeled by adding the NH_2 group to CQD-24 (**Figure 3b**). The calculation results show that the UV-Vis absorption opportunities are in the range of 140-230 nm. The absorption peak is at a wavelength of 184 nm. This absorption peak shifted to the right from the UV-Vis absorption peak without adding NH_2. The absorption of the UV-Vis spectrum also has the opportunity to occur for the wavelength range 240-340 nm, and the peak occurs at 246 nm. After the addition of NH_2, there was a broadening of the peaks in the 240-340 nm range. The second CQD model has a larger size (CQD-54) (**Figure 3d**) by adding the NH_2 group, which has been successfully calculated. The results obtained have a UV-Vis absorption spectral pattern in the wavelength range of 240-350 nm with peaks of 264 nm and 350-470 nm. CQD 54-NH_2 has two maximum UV-Vis absorption peaks at 396 nm and 441 nm in the 350-470 nm absorption range. The results of this calculation are under previous research that has been done [27]. From the calculation results, there is a suitability for the occurrence of a peak shift due to the addition of urea. The results show the same trend between the experiment and calculation; that is, with the addition of urea, there is a shift in the absorption peak (redshift). The effect of adding NH_2 is that the greater the amount of NH_2 on the CQD surface, the more electrons the CQD receives, resulting in more new molecular orbitals around the HOMO-LUMO, which causes the energy gap to decrease [28].

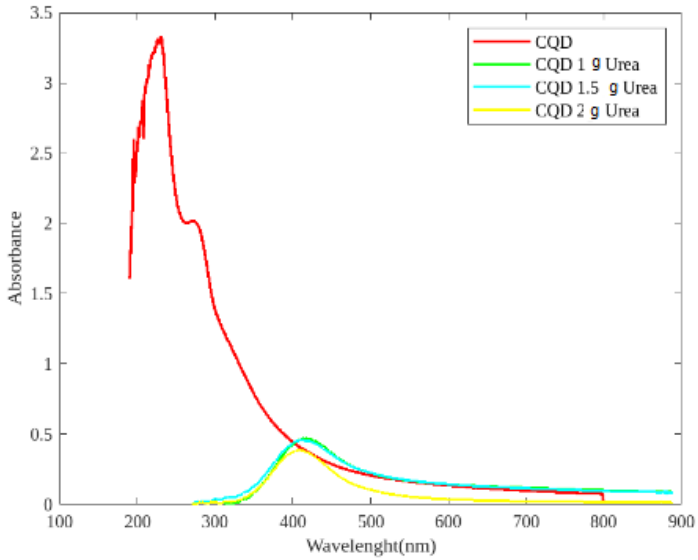
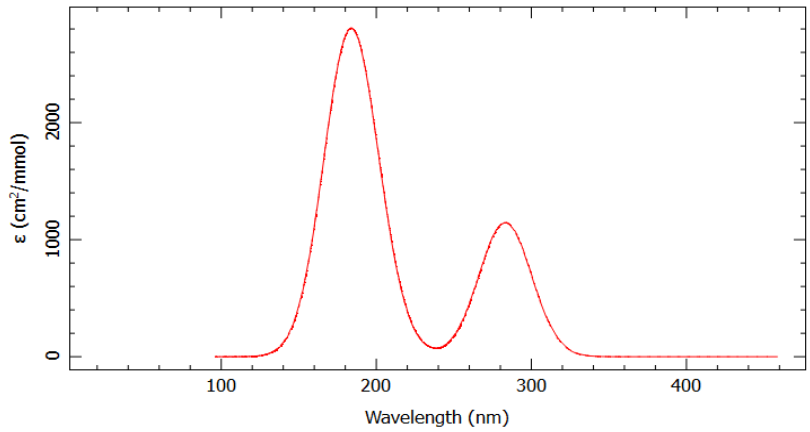
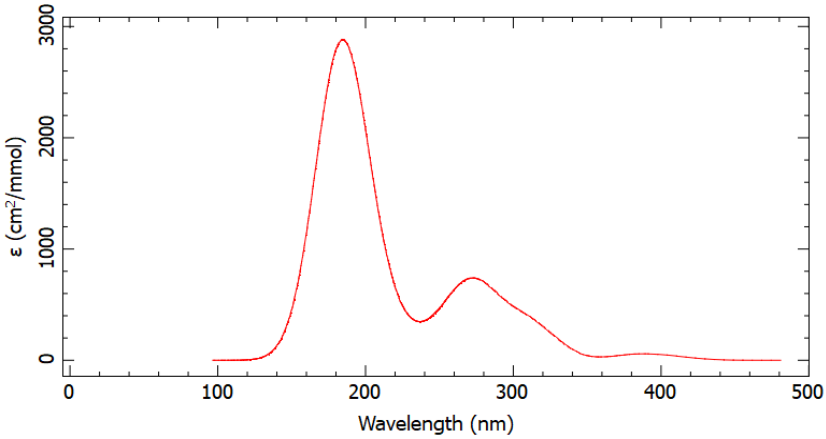


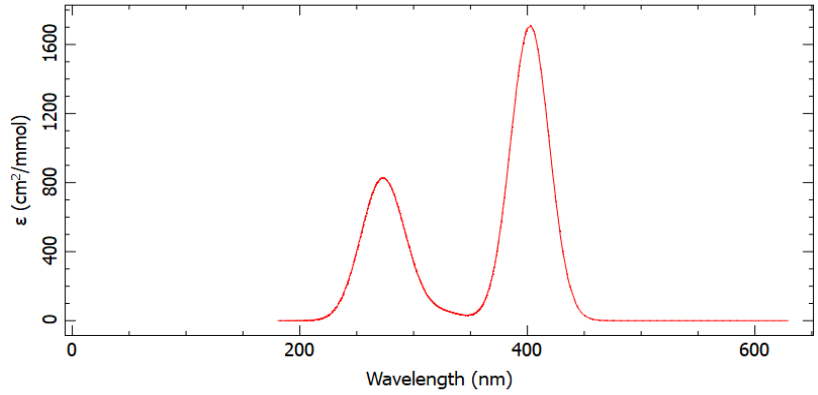
Figure 2. UV-Vis spectrum of Carbon Quantum Dots derived from mustard leaves with the addition of variations of urea grams



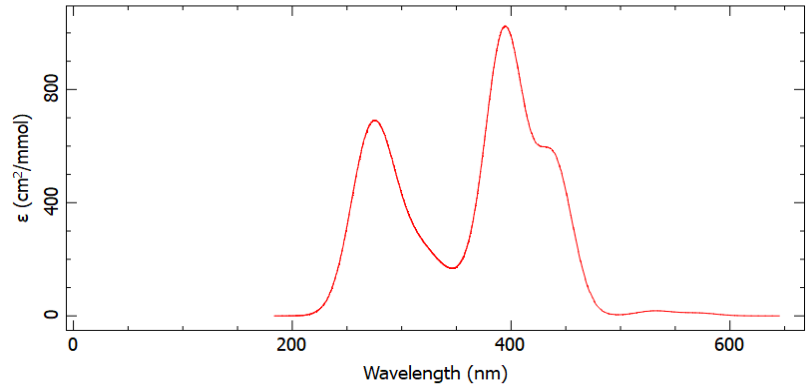
(a)



(b)



(c)



(d)

Figure 3. UV-Vis absorption spectra by TD-DFT calculations (a) CQD24 (b) CQD24-NH_2 (c) CQD54 and (d) CQD54-NH_2

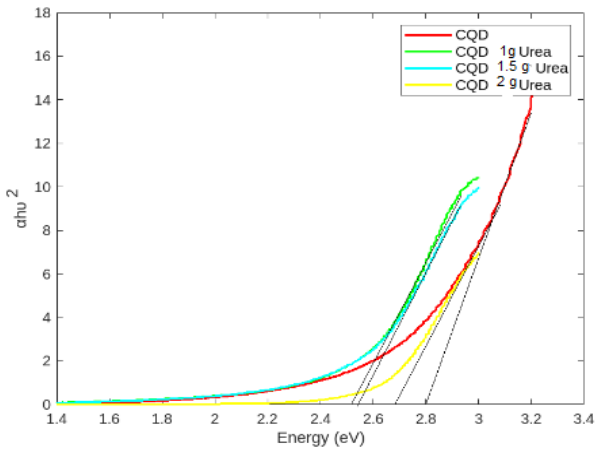


Figure 4. The indirect energy gap on the carbon quantum dot comes from mustard greens with the addition of a variety of grams of urea

The results of the gap energy calculation experimentally can be seen in **Figure 4**. The red line plot shows the gap energy for CQD without adding urea. CQD without urea has a gap energy of 2.8 eV. The CQD obtained by adding 1 g of urea is shown in **Figure 4** for the green line plot. The gap energy for CQD with adding 1 g of urea is 2.5 eV. The gap energy for CQD with adding 1.5 g urea is shown in **Figure 4**, the blue line plot. Calculation results were obtained for the energy gap of adding 1.5 g urea of 2.57 eV. Gap energy for CQD with adding 2 g of urea was obtained at 2.6 eV. The yellow line plot in **Figure 4** shows this gap energy.

Computational calculations are performed, and variations of the CQD model are calculated as geometric optimization. The optimization process will obtain a change in the location of the coordinates (x,y,z) to a new position (x',y',z') for each atom. This optimization aims to obtain a stable molecular geometric structure. The CQD-24-NH_2 model before optimization had a C-N bond length of 1.388 Å. After optimization the bond length became 1.390 Å. Likewise, for the CQD-54-NH_2 model, before optimization the C-N bond length was 1.391 Å, but after optimization the C-N bond length became 1.389 Å. **Figure 5a** shows the optimized CQD with 24 carbon atoms. **Figure 5b** shows the optimized CQD with 54 carbon atoms. The CQD model with the addition of NH_2 is shown in **Figure 5c** CQD24-NH_2 and **Figure 5d** CQD-54-NH_2, which has been optimized.

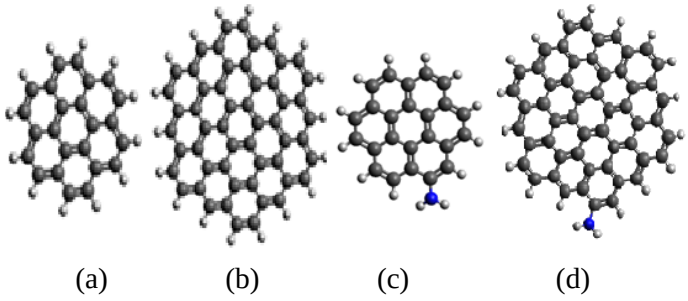


Figure 5. The optimized molecular structure of (a) CQD-24, (b) CQD-54 (c) CQD-24-NH_2 and (d) CQD-54-NH_2

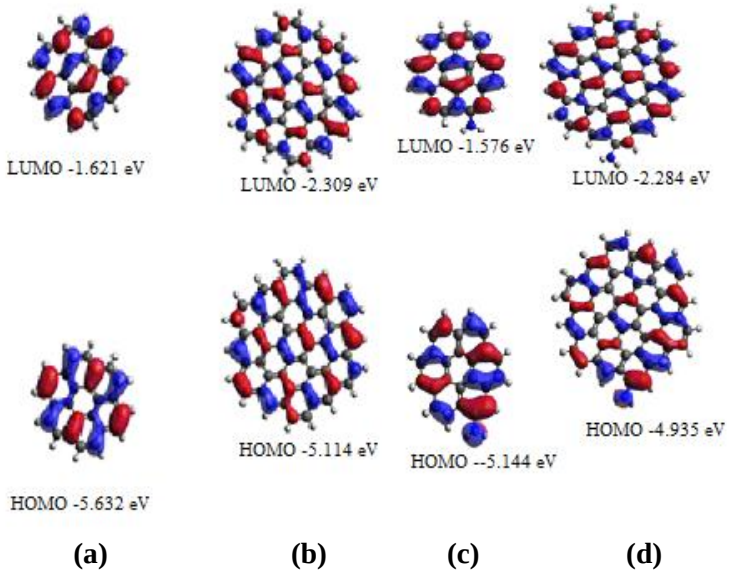


Figure 6. Molecular structures and orbital HOMO-LUMO (a.) CQD -24, (b.) CQD-54 (c.) CQD-24-NH_2 and (d.) CQD-54-NH_2

After the model has been optimized, the distribution of electrons in the molecular orbitals is calculated to obtain variations in the HOMO-LUMO energy levels. After the HOMO-LUMO energy levels in the CQD variation (**Figure 6**) are known, the difference in HOMO-LUMO energy levels (energy gap) can be seen (**Table. 1**). This aims to determine the molecular electronic properties of CQD. The calculation results show that the CQD-24 energy gap is 4.01 eV, and the CQD-54 energy gap is 2.81 eV. The calculation results show that the smaller the size of the CQD, the greater the gap energy. The computational CQD-54 gap energy has almost the same value as the CQD gap energy without adding urea to the experimental results. By adding the NH_2 group to CQD, the CQD-24-NH_2 energy gap is 3.50 eV, and the CQD-54-NH_2 energy gap is 2.65 eV. These results indicate that adding NH_2 lowers the gap energy in CQD-24 and CQD-54. Decreasing the energy gap is also appropriate and occurs experimentally. The calculated CQD-54-NH_2 energy gap has a value (2.65 eV) that is close to CQD addition of 1 g, 1.5 g, and 2 g urea from the experimental results (2.50 eV, 2.57 eV, and 2.60 eV). The energy levels of the highest occupied molecular orbital (HOMO) and lowest unoccupied molecular orbital (LUMO) in carbon quantum dots (CQD) allow them to be effective sensitizers in dye-sensitized solar cells (DSSCs). When exposed to sunlight, CQDs can inject electrons across the dye/semiconductor interface into the titanium dioxide (TiO_2) semiconductor. These injected electrons are then replenished by the electrolyte ($I^{3-}/I-$), which acts as an electron donor. This electron injection and transfer process contributes to the efficient conversion of sunlight into electricity in DSSCs [29].

This study obtained the results of the synthesis of CQD without urea and the addition of urea. The result emits a green light. These results can be seen in **Figure 7**. The results obtained are in accordance with previous research; CQD was synthesized by the microwave method. It can emit yellow–green and green color fluorescence under UV light (365 nm). The resulting particle size is around 2-6 nm.[29]. The photoluminescence (PL) origin of carbon quantum dots (CQDs) is explained by three main viewpoints: surface-state emission, core-state emission (quantum confinement), and molecular fluorescence. Surface-state emission is determined by hybridizing the carbon backbone and connected chemical groups. In nearly perfect carbon crystal regions with fewer defects and modified groups, core-state emissions arise from quantum confinement effects. Molecular fluorescence is induced by fluorescent impurities formed during synthesis. CQDs' PL behavior and quantum yield (QY) can be influenced by their particle size, surface states, heteroatom doping, and surface functionality. For example, as the size of the dot increases, the emission wavelength red-shifts, and the fluorescence intensity decreases. Additionally, heteroatom doping and changes in surface functional groups can also control the PL intensity [30].

Table 1. The comparison of gap energy CQD from the experiment result and computation analysis.

	Energy LUMO (eV)	Energy HOMO (eV)	Energy Gap (eV)
CQD			2.80
CQD 1.0 gr Urea			2.50
CQD 1.5 gr Urea			2.57
CQD 2.0 gr Urea			2.60
CQD24	-1.621	-5.632	4.01
CQD24- NH_2	-1.576	-5.144	3.50
CQD54	-2.309	-5.114	2.81
CQD54- NH_2	-2.284	-4.935	2.65

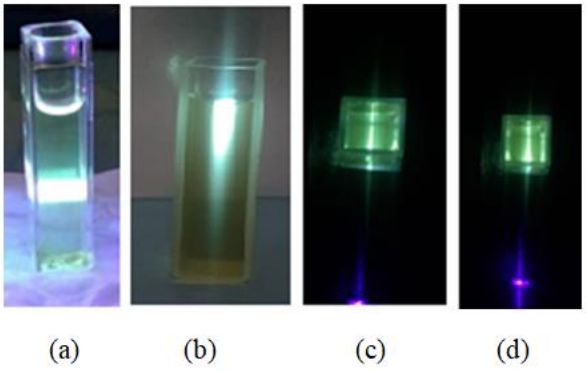


Figure 7. Presentation of the synthesis of CQD from mustard green (*Brassica juncea L*) leaf with the microwave treatment and visible green emission under UV; and (a) CQD, (b)CQD 1g urea (c)CQD-1.5 g urea (d) CQD 2 g urea

4. CONCLUSIONS

This research succeeded in synthesizing environmentally friendly CQD, through microwave irradiation of Mustard leaf *(Brassica juncea L*) with the addition of urea as a precursor without adding urea for synthesis. The optical properties of the CQD synthesis results have a UV-Vis CQD absorption spectrum (without the addition of urea) in the absorption range of 200-400 nm and a maximum absorption intensity at a wavelength of 233 nm. UV Vis CQD spectra with the addition of urea (1 g, 1.5 g, and 2 g CQD urea) have maximum absorption peaks at 424 nm, 422

nm, and 418 nm. The addition of urea causes a shift in the peak of the UV-Vis absorption spectrum towards red wavelengths (redshift). The results show similar trends between experiments and calculations; that is, with the addition of urea, there is a shift in the absorption peak (redshift). In addition, CQD from Mustard leaves (*Brassica juncea L*) with the addition of urea precursors without the addition of urea having carbon quantum dots (CQD) allows it to be an effective sensitizer in dye-sensitive solar cells (DSSCs). The addition of urea in the synthesis decreases the energy gap. These properties can be applied as needed. Since synthesized CQDs can emit yellow-green light, this property is suitable for use as optoelectronic and bioimaging devices.

ACKNOWLEDGMENTS

Authors thank PUSAT PENELITIAN DAN PENERBITAN (PUSLITPEN)—LP2M UIN Syarif Hidayatullah Jakarta for financial support BOPTN 2019. The authors also thank Pusat Laboratorium Terpadu (PLT) UIN Syarif Hidayatullah Jakarta and Theory Laboratory Physics Department IPB.

REFERENCES

1. Rani UA, Ng LY, Ng CY, Mahmoudi E. A review of carbon quantum dots and their applications in wastewater treatment. *Adv Colloid Interface Sci*. 2020;278:102124. doi:10.1016/j.cis.2020.102124

2. Guo X, Zhang H, Sun H, Tade MO, Wang S. Green Synthesis of Carbon Quantum Dots for Sensitized Solar Cells. *ChemPhotoChem*. 2017;1(4):116-119. doi:10.1002/cptc.201600038

3. Kumar P, Bhatt G, Kaur R, Dua S, Kapoor A. Synthesis and modulation of the optical properties of carbon quantum dots using microwave radiation. *Fullerenes Nanotub Carbon Nanostructures*. 2020;28(9):724-731. doi:10.1080/1536383X.2020.1752679

4. Hu X, Li Y, Xu Y, et al. Green one-step synthesis of carbon quantum dots from orange peel for fluorescent detection of Escherichia coli in milk. *Food Chem*. 2021;339(July 2020):127775. doi:10.1016/j.foodchem.2020.127775

5. Yu Z, Zhang L, Wang X, He D, Suo H, Zhao C. Fabrication of ZnO/carbon quantum dots composite sensor for detecting no gas. *Sensors (Switzerland)*. 2020;20(17):1-11. doi:10.3390/s20174961

6. Dager A, Baliyan A, Kurosu S, Maekawa T, Tachibana M. Ultrafast synthesis of carbon quantum dots from fenugreek seeds using microwave plasma enhanced decomposition: application of C-QDs to grow fluorescent protein crystals. *Sci Rep*. 2020;10(1):1-15. doi:10.1038/s41598-020-69264-9

7. Abu N, Chinnathambi S, Kumar M, et al. Development of biomass waste-based carbon quantum dots and their potential application as non-toxic bioimaging agents. *RSC Adv*. 2023;13(40):28230-28249. doi:10.1039/d3ra05840a

8. Huang P, Xu S, Zhang M, Zhong W, Xiao Z, Luo Y. Green vegetables derived simultaneously carbon dots as sensitizer and carbon particles as counter electrode for dye-sensitized solar cells. 2019;(February 2020):26. doi:10.1117/12.2539530

9. Arumugham T, Alagumuthu M, Amimodu RG, Munusamy S, Iyer SK. A sustainable synthesis of green carbon quantum dot (CQD) from Catharanthus roseus (white flowering plant) leaves and investigation of its dual fluorescence responsive behavior in multi-ion detection and biological applications. *Sustain Mater Technol*. 2020;23:e00138. doi:10.1016/j.susmat.2019.e00138

10. Song Y, Zhang M, Yin L, et al. Since January 2020 Elsevier has created a COVID-19 resource centre with free information in English and Mandarin on the novel coronavirus COVID- 19 . The COVID-19 resource centre is hosted on Elsevier Connect , the company ' s public news and information. *Int J Antimicrob Agents*. 2020;56(January):1-9. https://ejournal.unesa.ac.id/index.php/jurnal-kesehatan-olahraga/article/view/34491

11. Synthesis and analysis of Carbon Dots (CDs) from natural sources. In: *Empowering Science and Mathematics for Global Competitiveness*. ; 2019:5.

12. Rasal AS, Yadav S, Yadav A, et al. Carbon Quantum Dots for Energy Applications: A Review. *ACS Appl Nano Mater*. 2021;4(7):6515-6541. doi:10.1021/acsanm.1c01372

13. He P, Shi Y, Meng T, et al. Recent advances in white light-emitting diodes of carbon quantum dots. *Nanoscale*. 2020;12(8):4826-4832. doi:10.1039/c9nr10958g

14. Xue H, Yan Y, Hou Y, Li G, Hao C. Novel carbon quantum dots for fluorescent detection of phenol and insights into the mechanism. *New J Chem*. 2018;42(14):11485-11492. doi:10.1039/c8nj01611a

15. Ambrusi RE, Arroyave JM, Centurión ME, et al. Density functional theory model for carbon dot surfaces and their interaction with silver nanoparticles. *Phys E Low-Dimensional Syst Nanostructures*. 2019;114. doi:10.1016/j.physe.2019.113640

16. Bursch M, Mewes JM, Hansen A, Grimme S. Best-Practice DFT Protocols for Basic Molecular Computational Chemistry**. *Angew Chemie - Int Ed*. 2022;61(42). doi:10.1002/anie.202205735

17. Gelfand N, Freidzon A, Vovna V. Theoretical insights into UV–Vis absorption spectra of difluoroboron β-diketonates with an extended π system: An analysis based on DFT and TD-DFT calculations. *Spectrochim Acta - Part A Mol Biomol Spectrosc*. 2019;216:161-172. doi:10.1016/j.saa.2019.02.064

18. Yashwanth HJ, Rondiya SR, Dzade NY, Dhole SD, Phase DM, Hareesh K. Enhanced photocatalytic activity of N, P, co-doped carbon quantum dots: An insight from experimental and computational approach. *Vacuum*. 2020;180(July):109589. doi:10.1016/j.vacuum.2020.109589

19. Tiwari S, Talreja S. Green Chemistry and Microwave Irradiation Technique: A Review. *J Pharm Res Int*. 2022;34:74-79. doi:10.9734/jpri/2022/v34i39a36240

20. Fahyuan HD, Deswardani F, Nurhidayah N, et al. The effect of doping variation on band gap energy and crystal structure of Biochar/TiO2 thin layer. *J Phys Conf Ser*. 2021;1731(1). doi:10.1088/1742-6596/1731/1/012060

21. Yuniarti E, Nurlaela A. Komunikasi Fisika Indonesia Studi Komputasi Karakteristik Optik Cyanidin sebagai Sensitiser dengan Pelarut Ethanol, Air , dan Acetonitrile. 2023;20(1):39-48. doi:10.31258/jkfi.20.1.39-48

22. Azargoshasb T, Parvizi R, Bozorgzadeh F, Navid HA, Heidari H. Smart green CQD@SiO2 hybrid coated optical fiber manifesting dual versatile absorptive and MIP features towards epinephrine detection. *Nanoscale Adv*. 2022;5(2):459-470. doi:10.1039/d2na00687a

23. Alam AM, Park BY, Ghouri ZK, Park M, Kim HY. Synthesis of carbon quantum dots from cabbage with down- and up-conversion photoluminescence properties: Excellent imaging agent for biomedical applications. *Green Chem*. 2015;17(7):3791-3797. doi:10.1039/c5gc00686d

24. Architha N, Ragupathi M, Shobana C, et al. Microwave-assisted green synthesis of fluorescent carbon quantum dots from Mexican Mint extract for Fe3+ detection and bio-imaging applications. *Environ Res*. 2021;199(April):111263. doi:10.1016/j.envres.2021.111263

25. Kanagathara N, Bhavani R, Lo AY, Marchewka MK, Janczak J. Structural, vibrational characterization and DFT calculations of urea: DL-malic acid (1:1) – co-crystal. *J Mol Struct*. 2022;1270(August). doi:10.1016/j.molstruc.2022.133930

26. Langer M, Paloncýová M, Medveď M, et al. Progress and challenges in understanding of photoluminescence properties of carbon dots based on theoretical computations. *Appl Mater Today*. 2021;22:1-64. doi:10.1016/j.apmt.2020.100924

27. Umami R, Permatasari FA, Sundari CDD, Muttaqien F, Iskandar F. Surface Functional Groups Effect on the Absorption Spectrum of Carbon Dots: Initial TD-DFT Study. *J Phys Conf Ser*. 2022;2243(1). doi:10.1088/1742-6596/2243/1/012043

28. Hashemi D, Ma X, Ansari R, Kim J, Kieffer J. Design principles for the energy level tuning in donor/acceptor conjugated polymers. *Phys Chem Chem Phys*. 2019;21(2):789-799. doi:10.1039/c8cp03341b

29 . Yu T, Wang H, Guo C, Zhai Y, Yang J, Yuan J. A rapid microwave synthesis of green-emissive carbon dots with solid-state fluorescence and pH-sensitive properties. R Soc Open Sci. 2018;5(7). doi:10.1098/rsos.180245

30. Vercelli B. The role of carbon quantum dots in organic photovoltaics: A short overview. *Coatings*. 2021;11(2):1-26. doi:10.3390/coatings11020232