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Simulation of Optical Energy Gap for Synthesis Carbon Quantum Dot by Laser Ablation

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Abstract

Fluorescent Carbon Quantum Dots (CQD_S) are a new kind of carbon nanoparticles that have appeared recently and have collected much interest as potential competitors to conventional semiconductor quantum dots (QD_s). In addition to their comparable fluorescent properties, CQD_s have the desired specifications of environmental friendliness, low toxicity, simple synthetic routes, low cost and surface passivation The functionalization of CQDS allow the control of their physicochemical properties. The main aim of this kind of researches is to account the variables that cannot be measured directly from practical experiments. Therefore, the work here is focused on the account energy gap of bulk (Eg_{bulk}) by theoretically method (simulation) after taking other values that have been measured experimentally, so we can set an important database for these values which can be taking will be using form by researchers in this field in the future.

Keywords: Carbon quantum dots (CQDs), laser ablation in liquid (LAL), energy gap.

توظيف المحاكاة الحاسوبية لحساب قيمة فجوة الطاقة بتقنية الكاربون المكمم النقطي

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الخلاصة

النقاط الكمومية الكربونية المتفلورة هي نوع جديد من المواد النانوية الكربونية التي ظهرت مؤخراً وحظيت باهتمام كبير كمنافس محتمل على النقاط الكمومية التقليدية لأشباه الموصلات (QDs). وبالإضافة إلى خصائص الفلورة للكربون النقطي، فإن لديه المواصفات المطلوبة من صداقته للبيئية، وسميتة المنخفضة، وطريقة تحضيره البسيطة وتكلفتة المنخفضة. وتسمح خاصية الشد السطحي لهذه النقاط بالتحكم في خصائصه الفيزيائية الكيميائية. إن الهدف الرئيسي لهذا النوع من الأبحاث هو حساب المتغيرات التي لا يمكن قياسها مباشرة من التجارب العملية. لذلك، يركز العمل هنا على فجوة الطاقة Eg_{bulk} في الحساب نظرياً (اجراء محاكاة حاسوبية) بعد أخذ قيم أخرى تم قياسها تجريبياً. لذلك يمكننا ضبط قاعدة بيانات هامة لهذه القيم التي يمكن الاستفادة منها من قبل الباحثين في هذا المجال في المستقبل.

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Introduction

Semiconductor nanoparticles, especially QD_S are a zero-dimensional of holes Electrons in a small box which invite the effect of quantum confinement, have attracted great attention due to their individual chemical and physical characteristics which are dependent on the size of materials. Hence, there are many physical and chemical significant applications, for examples: light emitting diodes, an optical wave guide, solar cells, and photo catalysis. The quasi-continuous density of states in the conduction and the valence bands are split into discrete electronic levels, the spacing between these levels and the band gap (Eg) decreases with increasing particle size [1]. Moreover, for semiconductors, the band gap decreases when the particle size increases resulting to the conversion of energy bands into discrete molecular electronic levels [2]. In this system the carriers are confined in all directions in a quantum dot (QD_S) or quantum box [3]. Based on the ratio of confinement length (d) to the Bohr radius (r_B) of the exaction in bulk (d/r_B), there are two distinct regimes (charge carries confinement regime and the exaction confinement regime, when $d/r_B \gg 1$, the motion of exciton is not confined because the boundary condition, when $d/r_B \ll 1$ the number of excitons or bound states is formed due to the kinetic energies of the hole and the electron are larger than the Coulomb energy [4]. The wave function is squeezed because of the very strong confinement, the hole and the electron singly take up the less energy state in a confined potential [5]. An important property of quantum dots (QD_s) is its large surface area to volume ratio . The result of this advantage is that (QD_S) have obvious surface-related phenomena [6]. Laser ablation liquid is a versatile method capable of producing carbon quantum dots with size that is controlled according to the laser parameter like laser energy wavelength and pulse duration, [7]. Carbon quantum dots are typically quasi-spherical nanoparticles comprising amorphous to nanocrystalline cores with predominantly graphitic or turbo stratic graphene or carbon [8].

Experimental work

Synthesis of (CQDs) by Laser ablation in liquid was utilized using a pulsed Nd: YAG laser at1.064 μm and a repetition rate of 1 kHz for the production of carbon quantum dots. The graphite target in cylindrical form was placed on the bottom of a glass cuvette. The cuvette was filled with 3 mL of deionized water to produce carbon quantum dots, for laser energy (60) mJ at (2) min laser ablation time

Aim of the work

To find an energy gap of bulk by the Mat-lab software using experimental results

Experimental

Band gap measurement

The UV-Visible absorption spectrum of the synthesized CQDs was recorded in the wavelength region (100–900) nm. Figure-1 shows the optical absorption spectrum (UV) of the target in DIW, at laser energy (60 mJ) for 2 min.

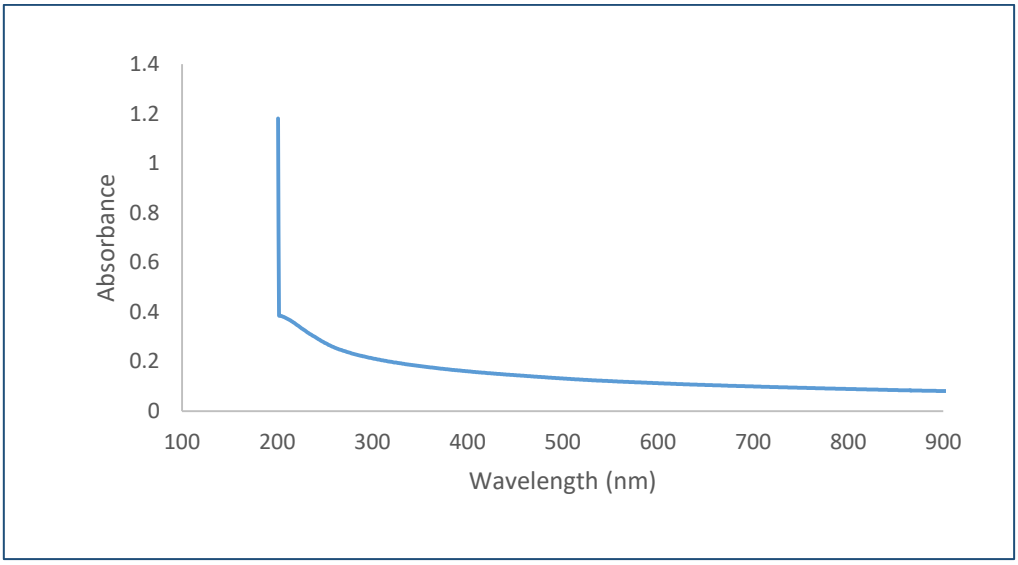

Figure 1-Absorbance spectrum of carbon quantum dots colloidal at 60 mJ for 2 min

After measurinr the absorbance using optima SP-3000 plus, double beam UV-VIS spectrometer was utilized to investigate the optical absorption spectra of carbon quantum dots colloids, this was done at ambient conditions employing quartz cell with optical path (1cm). From Figure-1 The optical direct energy gap (Eg_{QDS}) value was measured by the evaluation of the straight line of $(\alpha h\upsilon)^2$ plot against photon energy for the carbon quantum dots prepared at laser energy (60) mJ, (2) min laser ablation time, was equal to 3.1 eV for carbon quantum dots conductor, show in Figure-2.

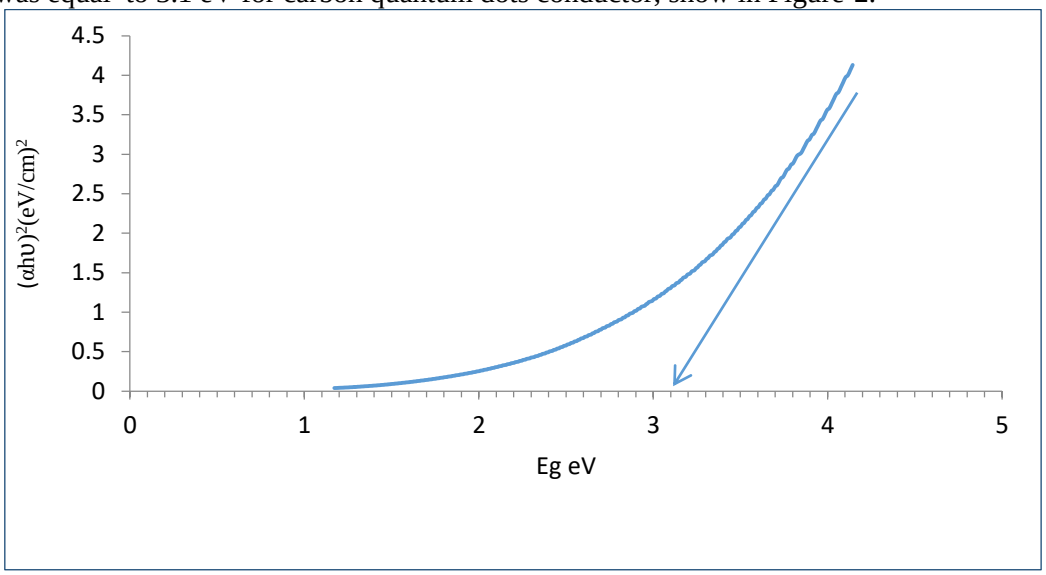

Figure 2- Optical band gap of CQDs at laser energy 60 mJ for 2 min.

Morphological characterization of CQDs suspension:

Figure-3 shows the spherical CQDs papered for a 2 min ablation time The size was changed from 1nm to 6nm (with an average size of 2 nm) and the large particle was changed to 14 nm and 16 nm.

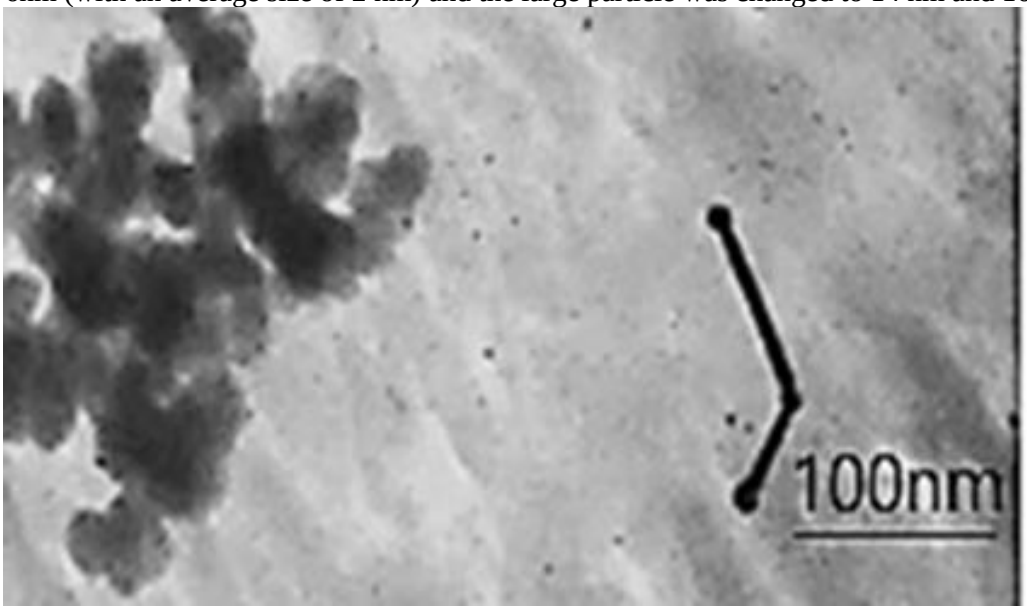

Figure 3-TEM image CQDs obtained at 60mJ for 2min.

X-ray Measurements

An accurate formation could be obtained by observing carbon quantum dots structure by X-ray (XRD) method. It is a very good mechanism employed to recognize the crystal-like phases that exist in materials and to observe the physical composition properties of these phases. The use of Scherrer's formula, equation (1), is an efficient method to evaluate the particle size by measuring the width of their diffraction curves [9]. Where δ is the crystal size, B is the half width, λ is the wavelength of the incident beam of the peak, and θ is the diffraction angle. Figure-4 clarifies the observation of the

carbon quantum dots prepared by laser ablation in liquid by X-ray diffraction (XRD) spectrum From the figure, a strong, sharp peak appears at an angle ($2\theta = 25.74^0$) and another peak at 43^0 related to the hexagonal carbon as a reflection from (002) and (100) planes. The XRD pattern of the peak is the reflections from (100) plane, of which is related to the structure of carbon with hexagonal phase (JCPDS Card 89-8487) [10].

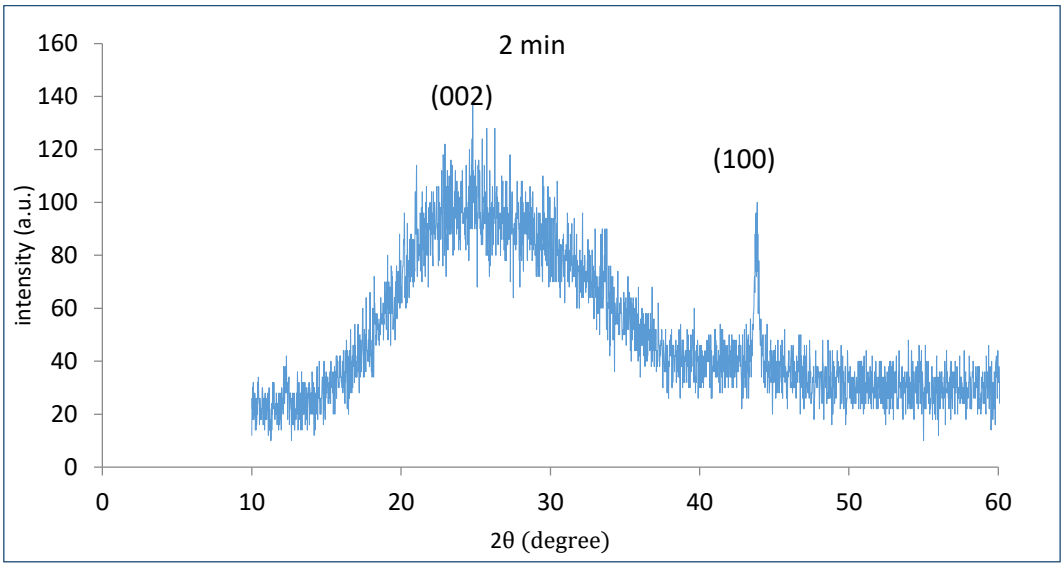

Figure 4- XRD diffraction of CQDs drop casted on glass.

From Figure-4, using Scherrer's formula, where K= 0.89, λ= 0.154 nm, $2\theta = 25.74^0$,the size of nanoparticle(δ) can be caculated

$$\delta = \frac{K\lambda}{\beta COS\theta} \quad (1)$$

$$\delta = 9.8nm$$

using this value the nanoparticle radius can be calculated from:

$$\delta = \pi R^3 \quad (2)$$

R=1.46 nm radius of nanoparticle.

Theoretical results:

Calculation of Energy bulk (Eg_{bulk})

As the particles become smaller, their electronic structure varies, so finally the charge carriers fabricate discrete energy states in the conduction and valence bands because of local confinement: there is not enough space for hole -electron pairs to shape. The optical and electronic properties of such very small particles are therefore more like those of a molecule than of an extended solid. Size effects are predictable to occur when the particle size becomes smaller than the Bohr radius (r_B) of the first exaction in the bulk semiconductor, the Bohr radius (r_B) is defined as [11]:

$$\boldsymbol{r_B} = \frac{\boldsymbol{h^2 \varepsilon_r \varepsilon_0}}{\boldsymbol{e^2}} \left(\frac{\boldsymbol{1}}{\boldsymbol{m_e^*}} + \frac{\boldsymbol{1}}{\boldsymbol{m_h^*}}\right) \quad (3)$$

Where, ε_r and ε_0 are the relative dielectric constants of material and the dielectric constants of the vacuum,respectively; h is the Plank constant ; e, $\boldsymbol{m_e^*}$ and $\boldsymbol{m_h^*}$ are the elementary charge, the electron mass and the effective mass of the charge carriers, respectively. Semiconducting nanoparticles with size smaller than r_B are described (QDs). In (QDs), the band gap energy becomes size dependent [12,13]:

$$Eg_{(QDS)} = Eg_{(bulk)} + \left(\frac{\boldsymbol{1}}{\boldsymbol{m_e^*}} + \frac{\boldsymbol{1}}{\boldsymbol{m_h^*}}\right) \frac{\boldsymbol{h^2}}{\boldsymbol{8R^2}} - \frac{\boldsymbol{1.82e^2}}{\boldsymbol{4\pi\varepsilon_0 R}} \quad (4)$$

First expression second expression third expression

The first expression is the band gap energy of the bulk semiconductor, the third expression shifts the energy gap of (QDs) to smaller energy as R, while the second expression shifts Eg ($_{QDs}$) to higher

energy as R^2. The third expression is very small. It is obvious that the band gap energy will always decrease As R gets larger. The values of energy gap and its radius from equations (1, 2) of the experimental work were used to find the value of energy gap of bulk theoretically using Mat-lab software , according to equation (4).

Conclusions

From the results we can conclude that laser energy leads to modification of the particle size and concentration of NPs in the solution. The band gap of quantum dots has decreased in comparison to the band gap of bulk because of the decrease of particles size according to equation (4).

References

1. Schön, G. and Simon, U. **1995.** A fascinating new field in colloid science: Small ligand-Stabilized metal clusters and their possible application microelectronics. *Colloid Polym. Sci*. **273**(3): 202-218.
2. Weller, H. **1993.** Quantized Semiconductor Particles: A novel state of matter for materials Science. *Adv. Mater*. **5**(2): 88-95.
3. Bowers, M., McBride, J. and Rosenthal, S. **2005**. White –light emission from magic-sized Cadmium Selenide nanocrystals, *J. Am. Chem. Soc*. **127**(44): 15378- 15379.
4. Anikeeva, P., Halpert, J., Bawendi, M. and Bulovic, V. **2007.** Electroluminescence from a Mixed Red-Green-Blue Colloidal Quantum Dot Monolayer, *Nano Lett*. **7**(8): 2196-2200.
5. Williams, L. and Adams W. **2007.** *Nanotechnology Demystified*, the McGraw-Hill Companies, USA.
6. DiMaio, J., Kokuoz, B. and Ballato, J. **2006**. White light emissions through downconversion of rare-earth doped LaF3 nanoparticles, *Optics Express*, **14**(23): 11412- 1417.
7. Xu, M., Li, Z., Zhu, X., Hu, N., Wei, H., Yang, Z. and Zhang, Y. **2013.** Hydrothermal Solvothermal Synthesis of Graphene Quantum Dots and Their Biological Applications. *Nano Biomedicine & Engineering*, **5**(2).
8. Shi, Y., Wei, S. and Zhiiang, G. **2014.** Carbon quantum dots and their applications. *Chem. Soc. Rev.***, 44**: 362-381
9. Ali, A. H., Shuhaimi, A., Hassan, Z. and Yusof, Y. **2013**. Compositional and Structural Characterization of Heterostructure InGaN-based Light- Emitting Diode by High Resolution X-Ray Diffraction, *J. of Advanced Materials Research*, **620**: 22-27.
10. Park, S. Y., Lee, H. U., Park, E. S., Lee, S. C., Lee, J. W., Jeong, S. W. and Lee, J**. 2014.** Photoluminescent green carbon nanodots from food-waste-derived sources: largescale synthesis, properties, and biomedical applications. *ACS applied materials and interfaces*, **6**(5): 3365-3370.
11. Gaponenko S. **2010.** *Introduction to Nanophotonics*, Cambridge University Press, Cambridge.
12. Khawla, S., Khashan, Ghassan M., Sulaiman, Rafal Mahdi. **2017**. Preparation of iron oxide nanoparticles-decorated carbon nanotube using laser ablation in liquid and their antimicrobial activity. *Artificial cells, nanomedicine, and biotechnology*.45(8): 1699-1709
13. Khawla, S., Khashan, Majid S., Jabir, Farah A., Abdulameer. **2019.** Carbon Nanoparticles Pre pared by Laser Ablation in Liquid Environment. *Surface Review and Letters*, DOI: 10.1142/S0218625X19500781.