

## **Development Simulation Model of Carbon Nanomaterial Quantum (CNQ) System: Fluorescence Carbon Nanomaterials (FCN)**

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**Abstract :** The use of fluorescence carbon nanomaterials (FCN) quantum yield in the simulation model by using MATLAB was highlighted since the simulation data generated with software is more accurate and precise than experimenting. The project conducted to determine carbon quantum dot (CQD) and FCN data, develop the coding graph of FCN in fluorescence emission system and simulate the combination graph of FCN by using MATLAB with FCN red, FCN yellow, FCN green and FCN blue. The development required a coding and MATLAB software to generate figure of each and combination graph of FCN's emission versus absorbance. The data shown the emission increase from FCN red ( $3.7848 \times 10^{20} \text{ nm}$ ), to FCN yellow ( $6.0438 \times 10^{20} \text{ nm}$ ), to FCN green ( $6.2981 \times 10^{20} \text{ nm}$ ), and lastly FCN blue ( $1.1878 \times 10^{21} \text{ nm}$ ). We can conclude that FCN blue and FCN green easier to yield. The quantum yield and size of particles also plays an important role to the emission rate of each FCN color. MATLAB proved that the graph generated was easy and smooth.

**Keywords:** Simulation, MATLAB Software, Carbon Quantum Dots, Fluorescence Carbon Nanomaterials.

### **1. Introduction**

The development simulation model of carbon nanomaterial quantum system using the basic coding of MATLAB. Quantum dots have some of benefits over different fluorescence compounds, which includes vibrant fluorescence, excessive optical stability, and resistance to metabolic degradation in organic applications [1]. FCN usually synthesized through nitric acid oxidation of carbon soot and this technique may be used for milligram scale synthesis. However, due to the lack of any established technique for the large-scale manufacture of FCNs, bulk synthesis remains a difficulty. As a result,

developing cost-effective and simple methods for producing highly luminous FCN on a large scale remains a significant issue [2].

The carbon nanomaterials selected was FCN red, FCN blue, FCN yellow and FCN green. Practically used MATLAB software to develop a better results resolution for a better discussion and comparison. The basic coding was applied to generate a graph simulation of absorbance versus emission intensity for FCN red, FCN blue, FCN green and FCN yellow. The data was collected from previous research done by Bhunia and his co-worker [3], with addition calculation.

The development of a coding in MATLAB software to generate figure of each and combination graph of FCN's emission versus absorbance are specified by using the C++ language. The data demonstrated an increase in the emission from FCN red ( $3.7848 \times 10^{20} \text{ nm}$ ) to FCN yellow ( $6.0438 \times 10^{20} \text{ nm}$ ) to FCN green ( $6.2981 \times 10^{20} \text{ nm}$ ) and lastly FCN blue ( $1.1878 \times 10^{21} \text{ nm}$ ). This indicated that FCN green and blue were simpler to yield. It's impossible to fathom how easily and smoothly the graph was generated on graph paper by hand.

### 1.1 FCN with emission intensity

FCN having 2-6 nm in length with a quantum yield of about ~3% had been synthesized through nitric acid oxidation of carbon soot and this technique may be used for milligram scale synthesis of that water-soluble debris. These FCN are nano-crystalline with a predominantly graphitic shape and suggest inexperienced fluorescence below UV (Ultra Violet) exposure.

Carbon nanoparticles, nanocrystals, nanotubes, fullerenes, nanofibers, graphene nanosheets, and porous carbon materials have potential applications in nanoelectronics [4], microelectrical devices, electrochemistry, sensors, catalysis, ultracapacitors, bioimaging, and drug delivery. FCN have recently gained prominence due to their exceptional photoluminescence characteristics [5]. Though FCNs produce some blue or green photoluminescence, [6] it is still relatively modest when compared to fluorescent carbon quantum dots.

The simulation of wavelength-emission intensity from previous research by Bhunia and his co-worker [3] only can be found in a sketch of graph without using the MATLAB in [7] results. The fluorescence is the emission of a photon from the lowest excited state ( $S_1$ ) to the ground state ( $S_0$ ) by a fluorophore. The photon's emission has a certain energy,  $E$ , and will thus be detected at a specific wavelength [8].

### 1.2 MATLAB Software

MATLAB was invented by mathematician and computer programmer Cleve Moler, Chonacky and Winch in 2005. His PhD work from the 1960s served as the inspiration for MATLAB. In 1967, he and his thesis advisor, George Forsythe, created the first version of MATLAB's linear algebra programming Chonacky and Winch, 2005 version. This was followed in 1971 by the Fortran code for linear equations.

MATLAB for short, is a multi-paradigm Moler, 1996, the high-performance programming language in technical computing [1]. It combines computing, visualization, and programming in a user-friendly environment in which problems and answers are stated in common mathematical notation. It is commonly used in math and computation, algorithm development, modeling, simulation, and prototyping, data analysis, exploration, and visualizations, scientific and engineering graphics, and application development, including the creation of graphical user interfaces Moler, 1996.

## 2. Software and Methods

The software used in this project was MATLAB by using basic coding C++ language. A device used this project was a laptop.

### 2.1 Methods

Firstly, the variables was determined to construct the graph. The constant is absorbance, the responding is emission intensity. Meanwhile the manipulated is the colour of FCN. Next, the coding needed to simulate the data can be refered at **Figure 2** and **Figure 3**. The coding was enter at live script and be runs for results. The simulation of graph appear.

## 2.2 Equations

The equations are used to calculate the data to generate a graph. The origin data obtained from the previous research and be modified by using the equations.

$$I_f(nm) = \Phi_f I_0(nm)(1 - 10^{-A}) \quad \text{Eq. 1}$$

$$A = -\log_{10} T \quad \text{Eq. 2}$$

$$T = \frac{I_1(nm)}{I_0(nm)} \quad \text{Eq. 3}$$

**Eq. 1** shows the formula to find the emission intensity with quantum yield ( $\Phi_f$ ), incident light intensity ( $I_0$ ) and power of absorbance ( $A$ ).

**Eq. 2** and **Eq. 3** are used to find the light incident intensity. **Eq. 2** is the formula to find the absorbance by negative log transmittance. Meanwhile, **Eq. 3** is the formula to find the transmittance by light emission divide the incident light.

## 3. Results and Discussion

### 3.1 Results

The absorbance was fixed at 1.0. These will result in the same distance for each color. The maximum peak of the FCN blue was  $2 \times 10^{21} \text{ nm}$ . It has been used as the maximum x-axis of the graph for the reference of differences between each graph of FCN. The emission intensity decreased to FCN green ( $6.2981 \times 10^{20} \text{ nm}$ ). Then, it decrease to  $6.0438 \times 10^{20} \text{ nm}$  for FCN yellow. FCN red emission intensity at  $3.7848 \times 10^{20} \text{ nm}$ , makes it the lowest among all the colors. Meanwhile, in the color FCN was plotted in one graph to compare the emission between each color. FCN red displays the lowest emission rate compared to other colors; FCN yellow, FCN green and, FCN blue.

The graphs show the absorbance of FCN against emission intensity. Since quantum yield refers to the effectiveness of the absorbed light into emission light, the absorbance and emission of the FCN was used as the variables.

### 3.2 Discussions

Based on the graph, the higher the Quantum Yields (QY) of the FCN, the higher the emission intensity. Even at low concentrations, a fluorophore with a high QY generates a lot of fluorescence. Effective blue and green emission photoluminescence (PL) has been recorded in various Carbon Dots systems up to this point [6], but effective red emission carbon dots are still rare [9].

Other than that, the size particles of the quantum yield also effect the emission intensity. This is because the quantum dots size can limit the energy at which electrons can exist in the particles. This means the particles can yield and absorb specific wavelengths of light depending on their size particle.

The procedure of graph simulation are interrupt by the full storage of the device. A toolbox of 'spline' are not able to install due to the full storage. It effects the shape of the graph. A curve graph couldnot be generated. But the linear graph formed allows a better differentiate.

**Table 1: Previous Research Data [3]**

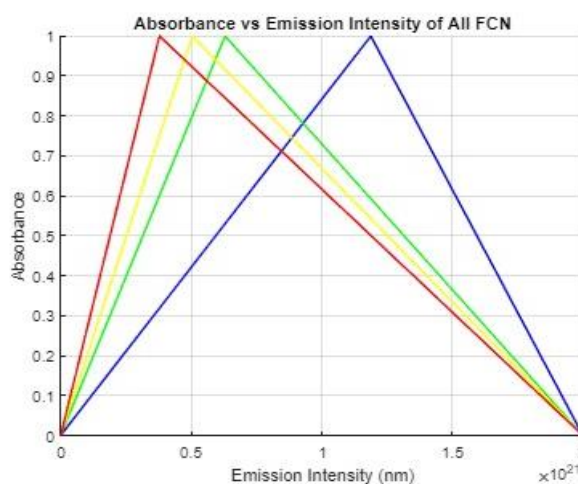
FCN	Absorbance	Size of Particles	Quantum yield (%)	Maximum Emission Intensity (nm)
Blue	1.0	400-2200 <i>Da</i>	6-30	440
Green	1.0	2-4 <i>nm</i>	14	500
Yellow	1.0	1-4 <i>nm</i>	12	560
Red	1.0	~4-10 <i>nm</i>	7	600

**Table 2: Emission Intensity of FCN**

FCN	Incident Light Intensity	Emission Intensity (a.u)	Emission Intensity (nm)
Blue	1.0	$7.94 \times 10^{-18}$	$1.1878 \times 10^{21}$
Green	1.0	$4.21 \times 10^{-18}$	$6.2981 \times 10^{20}$
Yellow	1.0	$4.04 \times 10^{-18}$	$6.0438 \times 10^{20}$
Red	1.0	$2.53 \times 10^{-18}$	$3.7848 \times 10^{20}$

**Table 1** shows the laboratory data obtained from the previous research done by Bhunia at his co-worker [3]. The absorbance, size of particles, quantum yield (%) and maximum emission intensity (nm) of each FCN color are recorded. The data will be used in the calculation process to obtain the emission intensity of FCN as shown in **Table 2**.

The result of simulation model were done in the MATLAB software. **Figure 1** is the simulation of combination graph of FCN red, blue, green and yellow versus absorbance. Meanwhile, **Figure 2** demonstrate the coding used to generate the combination graph of all FCN color. **Figure 3** shows the coding used to generate the graph of each FCN color. The combination of graph can be construct from a basic graph of each FCN that can be refered at **Figure 4**.



**Figure 1: Combination Graph of FCN**

```

clear all
clc
close all

x=[0; 1.1878*10^21; 2*10^21];
x1=[0; 6.2981*10^20; 2*10^21];
x2=[0; 5.0438*10^20; 2*10^21];
x3=[0; 3.7848*10^20; 2*10^21];
y=[0; 1; 0];

figure
hold on
plot(x,y, 'b')
% grid on
% xlabel('Emission Intensity (nm)')
% ylabel('Absorbance')
% title('Absorbance vs Emission Intensity of All FCN')
plot(x1,y, 'g')
% grid on
% xlabel('Emission Intensity (nm)')
% ylabel('Absorbance')
% title('Absorbance vs Emission Intensity of All FCN')
plot(x2,y, 'y')
% grid on
% xlabel('Emission Intensity (nm)')
% ylabel('Absorbance')
% title('Absorbance vs Emission Intensity of All FCN')
plot(x3,y, 'r')
hold off
grid on
xlabel('Emission Intensity (nm)')
ylabel('Absorbance')
title('Absorbance vs Emission Intensity of All FCN')

```

**Figure 2: Coding of Combination FCN Graph**

```

x=[0; 1.1878*10^21; 2*10^21];
x1=[0; 6.2981*10^20; 2*10^21];
x2=[0; 5.0438*10^20; 2*10^21];
x3=[0; 3.7848*10^20; 2*10^21];
y=[0; 1; 0];

figure
plot(x,y, 'b')
grid on
xlabel('Emission Intensity(nm)')
ylabel('Absorbance')
title('FCN Blue Emission')

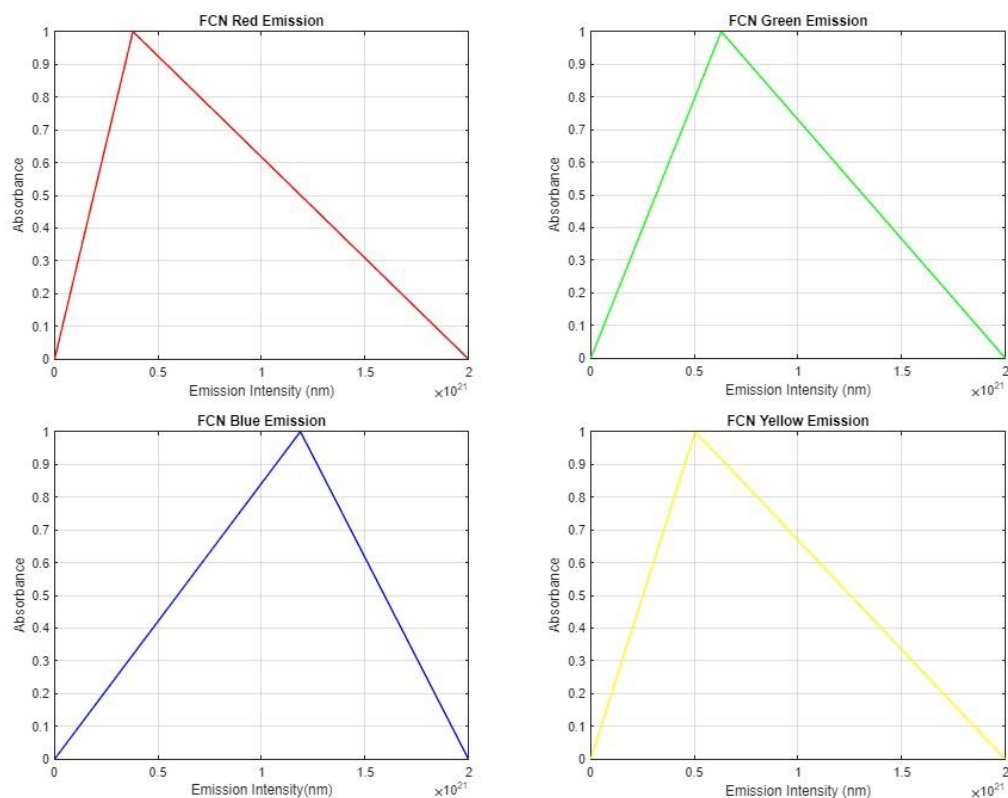
figure
plot(x1,y, 'g')
grid on
xlabel('Emission Intensity (nm)')
ylabel('Absorbance')
title('FCN Green Emission')

figure
plot(x2,y, 'y')
grid on
xlabel('Emission Intensity (nm)')
ylabel('Absorbance')
title('FCN Yellow Emission')

figure
plot(x3,y, 'r')
grid on
xlabel('Emission Intensity (nm)')
ylabel('Absorbance')
title('FCN Red Emission')

```

**Figure 3: Coding of Each FCN Graph**



**Figure 4: Graph of Each FCN**

#### 4. Conclusion

The FCN have a wide range of advantages especially in medical field such as biomedical image processing and signal processing, biosensor, and also in therapeutic application. The MATLAB image processing approach is an efficient solution for resolving image processing problems. Algorithms and mathematical process operations were implemented. This software also helps out with building out the complex algorithm stack [10] that can be use to detect fluorescence track. Conclude that, the graph simulation are easier when using MATLAB software. The resolution and precise of result obtained leads to the accurate analysis of the experiment. The MATLAB should be practice to all students.

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