**Quantum Dots and Quantum Yield**

**Physical Chemistry II Lab**

**CHM4111L**

**Dr. Clark**

**1. Objective and Relation to Lecture**

Provide a brief description of the purpose of the experiment. What are you trying to achieve or learn?

**2. Introduction / Theory**

Quantum dots (QDs) are semiconductor nanocrystals that exhibit unique size-dependent optical and electronic properties due to quantum confinement effects. Among these, cadmium selenide (CdSe) quantum dots are widely studied for their applications in optoelectronics, bioimaging, and solar energy conversion. This laboratory experiment aims to analyze CdSe quantum dots using ultraviolet-visible (UV-Vis) spectroscopy and X-ray fluorescence (XRF) spectroscopy. Additionally, the quantum yield of the quantum dots will be determined to evaluate their efficiency in emitting light upon excitation. These measurements provide valuable insight into the structural and electronic properties of the quantum dots and their size-dependent behaviors.

The fundamental principle behind the fluorescence of QDs is governed by quantum mechanics. The energy of a photon can be described using the equation:

where:

* is the energy of the photon (in joules),
* is Planck's constant (6.626×10−34 J s)
* is the frequency of the photon (in hertz).

When a photon hits a quantum dot, it can be absorbed, raising an electron from the valence band to the conduction band, creating an excited state. The energy difference between the two states can be described by:

Upon returning to its ground state, the electron releases energy in the form of a photon, which has a lower energy and longer wavelength than the absorbed photon, according to the equation:

where:

* is the wavelength of the emitted light (in meters),
* is the speed of light in a vacuum (3.00×108 m/s
* is the frequency of the emitted light.

To quantify the efficiency of fluorescence in QDs, we can determine the quantum yield (), defined as the ratio of the number of photons emitted to the number of photons absorbed. The quantum yield can be calculated using the following equation:

where:

* is the number of emitted photons,
* ​ is the number of absorbed photons.

To experimentally determine the quantum yield of

QDs, we can use a combination of fluorescence spectroscopy and UV-Vis absorption measurements:

1. **Fluorescence Spectroscopy**: Measure the emission spectrum of the QDs under a defined excitation wavelength. The intensity of the emitted fluorescence (IemittedI\_{\text{emitted}}Iemitted​) can be recorded.
2. **UV-Vis Absorption**: Measure the absorption spectrum of the QDs to determine the absorbance at the excitation wavelength. The absorbance (AAA) is related to the number of absorbed photons by Beer's Law:

where:

* + ϵ is the molar absorptivity (in L⋅mol−1)
  + c is the concentration of the QDs (in moles per liter),
  + l is the path length of the cuvette (in centimeters).

Using these measurements, the quantum yield can be calculated with the following relationship:

where:

* ​ is the intensity of the fluorescence from a standard sample,
* ​ is the absorbance of the standard at the excitation wavelength,
* ​ is the absorbance of the QD sample at the same wavelength,
* is the known quantum yield of the standard.

Some key differences between CdSe in its normal crystal structure vs CdSe quantum dots:

| Property | Typical CdSe | CdSe Quantum Dot |
| --- | --- | --- |
| Energy Bands | Continuous | Discrete (quantized levels) |
| Crystal Structure | Wurtzite or Zinc Blende | Similar, with surface effects |
| Surface Effects | Negligible | Dominant, some distortion, unsatisfied bonds |
| Optical Properties | Fixed Bandgap | Tunable Bandgap (size-dependent) |
| Density of States | Continuous | Discrete |

**3. Materials and Equipment**

* 5 CdSe QD solutions
* Toluene
* UV-Vis Spectrophotometer
* Quartz Cuvettes

**4. Experimental Procedure**

Your CdSe quantum dot solutions have been prepared for you. There are 5 unknown solutions and 1 standard solution.

**Measurement of UV-Vis Absorption**

* + Use a UV-Vis Spectrometer to measure the absorption of your solutions.
  + Use a plastic pipette to transfer your QD solution into a quartz cuvette.
  + Your blank cuvette will be toluene.
  + After you complete each measurement, DO NOT DISPOSE OF THE QD SOLUTION. Pour each solution back into their original vials. It is very important to avoid cross-contamination, so keep track of your pipettes, and rinse the quartz cuvette with toluene in between each solution.
  + Note: quartz cuvettes are very fragile and very expensive. Handle them very carefully, be gentle when placing them in and out of the UV-Vis, and **do not break them**.

**Operating the UV-Vis:**

Open the LabX 2017 software on the computer and turn on the UV-Vis spectrometer. Select the method “Quantum Dots”, make sure it is highlighted, and click “Start” in the menu along the top of the screen (another button called “UV5BIO” will pop up and you may need to click this).

In the window that pops up, increase the number of samples to 1, and label your sample. Click “Start” in this window, and then click “Show Workbench” in the top left corner of the screen. Look in the upper left part of the workbench in “Tasks” and make sure that your task is the only one running.

Follow the prompts to measure your blank and your sample. Save your sample spectrum as a .csv file. (In the workbench window, above the generated spectrum, you should see four small icons. The furthest right is called “chart export”. Select this one and save as a .csv file).

Repeat the above procedure for all samples, labeling your spectra appropriately.

**7. Calculations and Analysis**