

# Investigation into Quantum States And Spectra: Gas Excitement and Optical Properties

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## Abstract

This experiment is designed to study the specific properties of various substances through their spectral profiles and absorbance rates. By exciting Mercury, it was found that the spectrometer had a lengthening effect on light by 19.8 nm. The accurate calibration of the spectrometer allowed for independent verification of Hydrogen's spectral lines and the spectral properties of Helium. It was also possible to independently identify Krypton by its spectral lines. The experimental relationship of transmittance and absorbance was confirmed with their theoretical relationship. Specifically, the yellow dye was assessed to be in the ideal range for the photovoltaic semiconductor properties.

## 1 Introduction

It is important to understand unique wavelength and the amount of emission energy from the spectra of the different energy states, as it explains the atomic behavior of specific atom which can be applied to various fields in engineering physics. By observing the emission spectra of atoms, we gain information on unique spectral lines at specific wavelengths for each energy transitions.

Max Planck suggested that electromagnetic energy is quantized and introduced the concept of Planck's constant in order to model the emission energy of a photon as a form of packet, represented as:

$$E = h\nu = \frac{hc}{\lambda} \quad (1)$$

Later, Balmer suggested an empirically obtained equation for the energy of the hydrogen atom's visible spectrum. The energy of an emitted photon of Balmer series is represented as:

$$E = hf = R_{EH} \left( \frac{1}{2^2} - \frac{1}{n^2} \right) [1] \quad (2)$$

For hydrogen-like atoms, with the assumption of single electron engaged, the energy can be expressed using Bohr's model as:

$$E_n = -\frac{Z^2 k_e e^2}{2n^2 a_0} \approx -\frac{13.6 Z^2}{n^2} \text{ eV} [1] \quad (3)$$

In this experiment, the behaviour of emission spectra will be analyzed for hydrogen-like atoms by comparing theoretical wavelengths with experimental wavelengths measured using a spectrometer (PS-2600). Any discrepancies and uncertainties between the theoretical and experimental results will be evaluated and explained.

Additionally, the transmittance, absorbance, and fluorescence of coloured dye solutions will be analyzed, as these measurements verify the specific wavelengths at which transitions occur across different visible colour ranges.

## 2 Materials and Methods

### 2.1 Materials

#### General Equipment:

- Spectrometer (Model: PS-2600)
- Spectrometry Software
- Gas discharge tubes
- Optical fiber cable
- Cuvette holder
- Distilled water (for calibration)
- Light source (for transmittance/absorbance measurements)

#### Specific Materials by Part:

- Part 1: Mercury gas discharge tube
- Part 2: Hydrogen gas discharge tube
- Part 3: Helium gas discharge tube
- Part 4: Unknown gas discharge tube
- Part 5: Cuvettes with blue, red, and green dye solutions
- Part 6: Cuvettes with yellow dye solutions

## 2.2 Methods

### General Setup for All Parts:

1. Turn on the spectrometer (PS-2600) and connect it to the spectrometry software.
2. Calibrate the spectrometer by clicking **CALIBRATE** in the software with distilled water inserted into the cuvette.

#### 2.2.1 Part 1: Calibration of the Spectrometer with a Mercury (Hg) Tube

1. Connect the mercury discharge tube to the power supply.
2. Position the fiber optics probe close to the mercury gas tube.
3. Start recording the emission spectrum using the spectrometry software and calculate the expected emission energy from the experimental wavelengths.

#### 2.2.2 Part 2: Helium Emission Spectra

1. Repeat the procedure from Part 1 using a helium gas discharge tube.
2. Compare the experimentally obtained wavelengths and emission energies with Equation (2) : Balmer series of hydrogen; and Equation (3) : Energy of stationary states of hydrogen-like atoms.

#### 2.2.3 Part 3: Helium Quantum State Transitions

1. Record the emission spectrum of helium, focusing on the spectral lines corresponding to the transition  $n = 3$  to  $m = 2$ .
2. Refer to Table 5 and convert the corresponding wavelengths of the spectral lines into energy.

3. Calculate the changes in the principal quantum number ( $\Delta n$ ), orbital angular momentum ( $\Delta l$ ), and total angular momentum quantum number ( $\Delta J$ ) for the observed transitions.

#### 2.2.4 Part 4: Determination of the Unknown Gas

1. Replace the discharge tube with the one containing the unknown gas.
2. Observe the wavelengths where the spectral lines peak and identify the gas by comparing the observed wavelengths to the reference values of known gases (refer to Appendix 2).

#### 2.2.5 Part 5: Transmittance and Absorbance Measurements

*Note: This part does not require gas tubes or probes. Only the spectrometer and cuvettes with solutions are needed.*

1. Insert a cuvette with distilled water and calibrate the spectrometer using the software.
2. Insert the cuvette with the blue dye solution and record the absorbance and transmittance.
3. Repeat the process with the red and green dye solutions.

#### 2.2.6 Part 6: Fluorescence

1. Insert a cuvette with the yellow dye.
2. Record the spectrum and observe it in the 405 nm to 500 nm range.
3. Use the experimental wavelength at the absorption edge to compute the band gap energy of the dye.

## 3 Data and Analysis

### 3.1 Spectrometer Calibration with Mercury

The measured intensity of light emitted by Mercury was recorded and displayed in Figure 1. The peaks were identified.

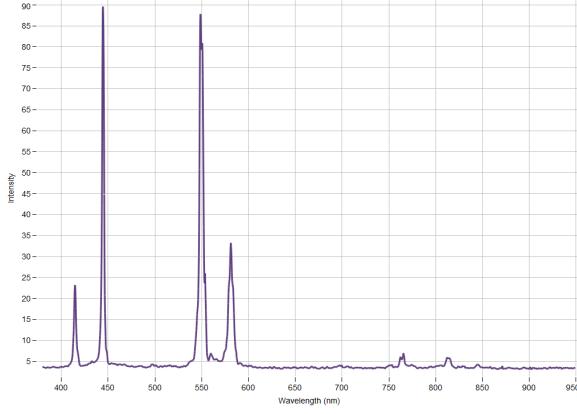


Figure 1: Experimentally measured intensity of emitted light from Mercury

The peak intensity wavelengths are compared in Table 1 to their expected wavelengths.

Expected $\lambda$	Experimental $\lambda$
405 nm	$414 \pm 3$ nm
408 nm	$414 \pm 3$ nm
436 nm	$444 \pm 3$ nm
546 nm	$548 \pm 3$ nm
577 nm	$581 \pm 3$ nm
579 nm	$583 \pm 3$ nm

Table 1: Expected intensity peaks and experimental intensity peaks at specific wavelengths ( $\lambda$ )

A linear regression model was generated using the experimental and expected wavelengths to calibrate the shift in wavelengths from the experimental devices.

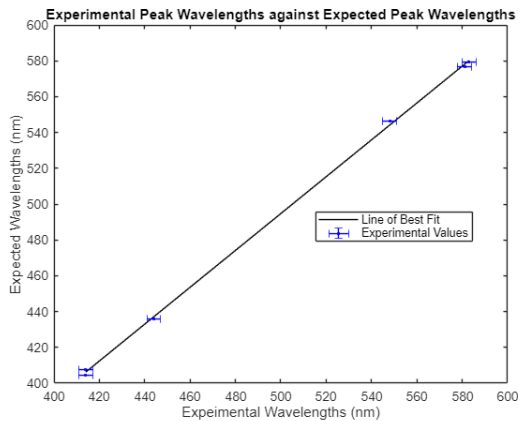


Figure 2: The plot displays the experimentally observed peak intensity wavelengths of mercury against the wavelengths where the peaks are expected, including the linear regression model

A linear regression model,  $\lambda_I(\lambda_E) = m\lambda_E + b$ , was found with a slope,  $m$ , of  $1.029 \pm 0.010$  and a vertical adjustment,  $b$ , of  $-19.8 \pm 4.8$ . The linear regression model was found to have an  $R^2$  of 0.9997. The  $R^2$  shows that 99.97% of the variation of the expected wavelengths is explained by the experimental wavelengths measured, strongly supporting the use of a linear regression model.

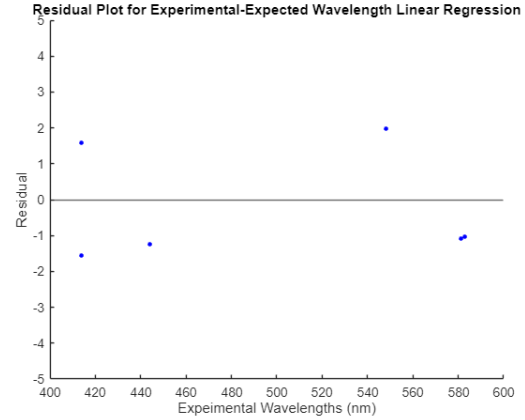


Figure 3: The plot shows the residuals of the linear regression for the expected and experimental peak intensity wavelengths

The linear regression model's residuals are small and appear to have a random scatter about the y-axis, further confirming the model's efficacy. Since this linear regression model is sufficient, we can calibrate the spectrometer reading accordingly.

The  $\chi^2_v$  is calculated to be 1.48, which indicates an underestimation of experimental uncertainties. The values from Table 1 were converted to their energy equivalents using  $E = \frac{hc}{\lambda}$ .

Expected Energy	Experimental Energy
3.064 eV	$2.995 \pm 0.044$ eV
3.041 eV	$2.995 \pm 0.044$ eV
2.845 eV	$2.792 \pm 0.038$ eV
2.271 eV	$2.262 \pm 0.024$ eV
2.149 eV	$2.134 \pm 0.022$ eV
2.141 eV	$2.126 \pm 0.022$ eV

Table 2: Energy of expected and experimental intensity peaks at specific wavelengths

The linear regression model of the expected and experimental energies,  $E_I(E_E) = nE_E + c$ , with a slope,  $n$ , of  $1.055 \pm 0.011$  and a vertical adjustment,  $c$ , of  $-0.106 \pm 0.029$

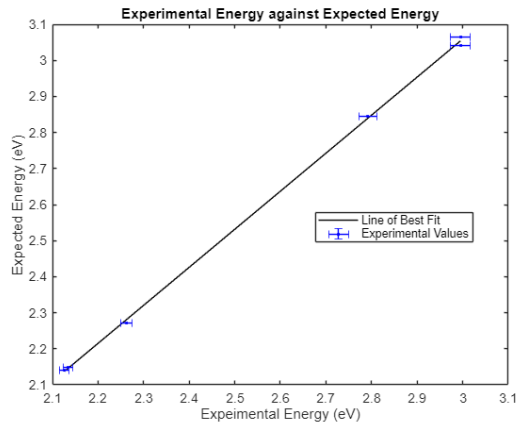


Figure 4: The plot displays the experimentally measured energy and the expected energy of the Mercury's emitted light with a linear regression model

The linear regression model has an  $R^2$  value of 0.9996, which means that 99.96% of the variation in the expected energy can be explained by the experimental energy, making this a highly effective model.

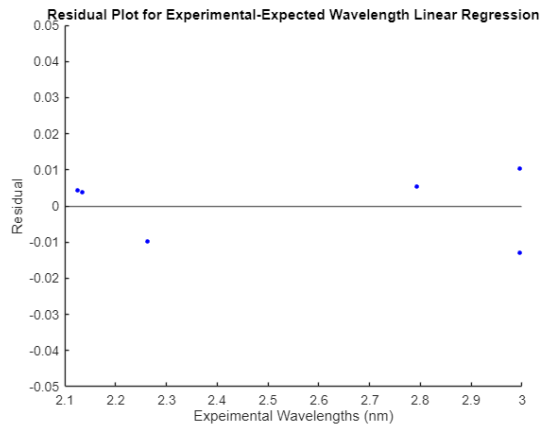


Figure 5: The plot shows the residuals for the linear regression of the expected and experimental energies

The residual plot shows a random scatter grouped around the y-axis, which implies that the linear regression is a good model. Further, the  $\chi^2_v$  for this model is 1.06, which suggests the uncertainties are reasonably estimated for the relationship. Using these models for the recorded data, it is known that a shift of -19.6 should be applied to recorded wavelengths to align them with true wavelengths. Therefore, it is known that the apparatus we are using makes records the wavelengths as approximately 19.6 nm longer than they are in

reality. This adjustment will make the subsequent readings more accurate.

### 3.2 Quantum State Energy of Hydrogen

Equation (3) calculates the energies of the quantum states of hydrogen. Equation (2) calculates the expected energy of the spectral lines. These values are reported in Table 3.

Q. Num.(n)	Quant. Energy	S.L. Energy
3	-1.511 eV	1.890 eV
4	-0.850 eV	2.551 eV
5	-0.544 eV	2.857 eV

Table 3: Q. Num. corresponds to the quantum number; the Quant. Energy corresponds to the energy of the quantum states; S.L. Energy corresponds to the expected energy of the spectral lines

The energy of the spectral lines can be converted to specific wavelengths, and the corresponding measured wavelength peaks are reported in Table 4.

Expected Wavelengths	Exptl. Wavelengths
656 nm	658 $\pm$ 3 nm
492 nm	486 $\pm$ 3 nm
434 nm	443 $\pm$ 3 nm

Table 4: The expected wavelengths of Hydrogen's strongest spectral lines and the recorded spectral lines

The measured wavelength peaks are near where the quantum numbers predict the expected wavelengths. However, two of the three peaks are outside of the uncertainty range, which would account for the equipment's uncertainty. This suggests additional error sources with varying effects depending on the wavelengths in question.

### 3.3 Quantum Energy, Transitions of Helium

#### 3.3.1 Analysis of Measured and Reference Wavelengths

The measured wavelengths ( $\lambda_{\text{exp}}$ ) deviate slightly from the reference wavelengths ( $\lambda_r$ ), with the largest difference being 10 nm and the smallest difference being 0.5 nm. Given that the spectrometer's uncertainty is  $\pm 3$  nm, the experimental wavelengths of the emission lines were slightly off from the theoretical values, but they remain within an acceptable range.

For the emission line corresponding to the transition from  $1s2p$  to  $1s^2$  (first column of Table 5), the spectrometer did not display a peak near 58 nm. This is because the operational range of the PS-2600 spectrometer is between 390 nm and 950 nm, which excludes this wavelength.

Initial State	Final State	Intensity	$\lambda_r$ (nm)
1s2p (1)	1s <sup>2</sup> (0)	1000	58.43339
1s3s (1)	1s2p (2)	200	706.5190
1s3p (1)	1s2s (1)	500	388.8648
1s3d (3)	1s2p (2)	500	587.5621
1s3d (2)	1s2p (1)	100	667.8151
1s3p (1)	1s2s (0)	100	501.56783
1s4d (1)	1s2p (2)	200	447.14802

Initial State	Final State	$\lambda_{exp} \pm$	$\lambda_r - \lambda_{exp}$
1s2p (1)	1s <sup>2</sup> (0)	N/A	N/A
1s3s (1)	1s2p (2)	706 $\pm$ 3	0.519
1s3p (1)	1s2s (1)	399 $\pm$ 3	-10.14
1s3d (3)	1s2p (2)	591 $\pm$ 3	-3.44
1s3d (2)	1s2p (1)	669 $\pm$ 3	-1.18
1s3p (1)	1s2s (0)	506 $\pm$ 3	-4.43
1s4d (1)	1s2p (2)	455 $\pm$ 3	-7.85

Initial State	Final State	$E_n$ (eV)	$E_m$ (eV)
1s2p (1)	1s <sup>2</sup> (0)	-21.221	-24.57
1s3s (1)	1s2p (2)	-1.755	-3.60
1s3p (1)	1s2s (1)	-3.189	-4.75
1s3d (3)	1s2p (2)	-2.110	-3.60
1s3d (2)	1s2p (1)	-1.857	-3.35
1s3p (1)	1s2s (0)	-2.472	-3.95
1s4d (1)	1s2p (2)	-2.773	-3.60

Initial State	Final State	$\Delta n$	$\Delta l$	$\Delta J$
1s2p (1)	1s <sup>2</sup> (0)	-1	-1	-1
1s3s (1)	1s2p (2)	-1	1	1
1s3p (1)	1s2s (1)	-1	-1	0
1s3d (3)	1s2p (2)	-1	-1	-1
1s3d (2)	1s2p (1)	-1	-1	-1
1s3p (1)	1s2s (0)	-1	-1	-1
1s4d (1)	1s2p (2)	-2	-1	1

Table 5: Electron configurations, emission lines, energy states, and selection rules for various transitions.

### 3.3.2 Spectral Lines and the Difference Between Helium and Hydrogen

In this experiment, there are five spectral lines corresponding to the transition of the helium atom from  $n = 3$  to  $m = 2$ . The reason why the He spectral lines differ from those of hydrogen is due to the number of electrons in each atom.

The hydrogen atom has only one electron, which results in a single specific energy transition from  $n = 3$  to  $m = 2$ . In contrast, helium atoms have two electrons that interact with each other, leading to electron-electron repulsion. This repulsion causes the splitting of energy levels, resulting in multiple spectral lines (five spectral lines as listed in Table 6 for the same  $n = 3$  to  $m = 2$

transition.

As seen in Table 6, one electron is located in the  $1s$  state, while the other electron is located in the  $n = 3$  state (either  $3s$ ,  $3p$ , or  $3d$ ). When this  $n = 3$ -located electron moves to  $n = 2$ , electron-electron repulsion occurs, slightly affecting the emitted energy. This results in multiple spectral lines.

Initial State	Final State
$1s3s$ (1)	$1s2p$ (2)
$1s3p$ (1)	$1s2s$ (1)
$1s3d$ (3)	$1s2p$ (2)
$1s3d$ (2)	$1s2p$ (1)
$1s3p$ (1)	$1s2s$ (0)

Table 6: Transitions of the Helium Atom from  $n=3$  to  $m=2$

### 3.3.3 Why Equation (2) and (3) are Not Applicable for Neutral Helium

The main difference between hydrogen-like ions and the neutral helium atom is the number of electrons. A  $\text{He}^+$  ion has only one electron, whereas a neutral helium atom has two electrons. Equation (2) is designed for hydrogen-like ions with a single electron. In a neutral helium atom, the repulsive force between the two electrons alters the energies of the spectral lines, making Equation (2) inapplicable for calculating the spectral lines of neutral helium.

Additionally, the wavelength calculated using Equation (3) is  $164 \pm 3$  nm, which significantly differs from the given  $\lambda \approx 588$  nm for the emission of the strongest peak of the helium atom. This discrepancy can be attributed to the nature of the Equation (3) where it assumes hydrogen-like atoms, meaning only one electron is involved, not two as in the case of neutral helium.

### 3.3.4 Selection Rules for Transitions

The selection rules governing the transitions observed in the experiment are as follows:

- $\Delta n$ : The principal quantum number difference does not affect the transitions directly; in this experiment, transitions from  $n = 3$  to  $m = 2$  were primarily observed.
- $\Delta l$ : The orbital angular momentum quantum number must change by 1, so  $\Delta l = \pm 1$ .
- $\Delta J$ : The total angular momentum quantum number must change by 0, 1, or -1, meaning

$$\Delta J = 0, 1, -1.$$

### 3.4 Determining Unknown Gas

The spectral emissions were collected from the unknown gas tube. Once collected, the spectral lines were identified and compared against known possible gases. It was determined that the gas observed most closely matched the spectral profile of Krypton.

Kr WvLngs	Exptl. WvLngs	Intensity
427 nm	N/A*	N/A*
432 nm	441±3 nm	0.0718
557 nm	562±3 nm	0.0894
587 nm	592±3 nm	0.0999
646 nm	N/A*	N/A*
759 nm	760±3 nm	1
769 nm	771±3 nm	0.924
810 nm	813±3 nm	0.804
826 nm	831±3 nm	0.487

Table 7: Expected wavelengths of the spectral line peaks and their experimental counterparts with their relative intensity to the maximum recorded intensity. \*The presence of the peak is unclear as the intensity is comparable to the noise of the experiment, so it cannot be determined

Despite some undetermined peaks due to the intensity of the noise in the experiment, given the possible options, it becomes sufficiently evident that the unknown gas in the tube is Krypton.

### 3.5 Transmittance and Absorbance

#### 3.5.1 Absorbance Calculations

The table below shows the transmittance and absorbance for blue, red, and green dye solutions. The absorbance values were calculated using  $A = -\log_{10}(T)$ , where  $T$  is the transmittance in percent. The software spectrometer automatically calculates the absorbance from the transmittance using this equation, and thus, the theoretical and experimental absorbance values are exactly the same, hence the experimental absorbance is not included in the table below.

Color	$\lambda_{\max}$ (nm)	$T_{\text{peak}}$ (%)	$A_{\text{theo}}$
Blue	606.4	6.034	1.219
Red	436.9	3.769	1.219
Green	433.2	3.896	1.409

Table 8: Transmittance and absorbance values at their peak for blue, red, and green dye solutions.

#### 3.5.2 Explanation of Colors in White Light

The blue dye has low transmittance (high absorbance) at 606.4 nm, which is in the red region of the spectrum. This indicates that the blue dye absorbs red light and transmits blue light, making it appear blue to the human eye. Similarly, the red dye has low transmittance at 436.9 nm, which falls in the blue and violet region. This suggests that the red dye absorbs blue and violet light while transmitting red light. The green dye has low transmittance at 433.2 nm (blue-violet region), allowing green light to be transmitted and appear green.

### 3.6 Fluorescence

The absorption spectra of the yellow dye cuvette were taken and reported from wavelengths of 350nm to 950nm.

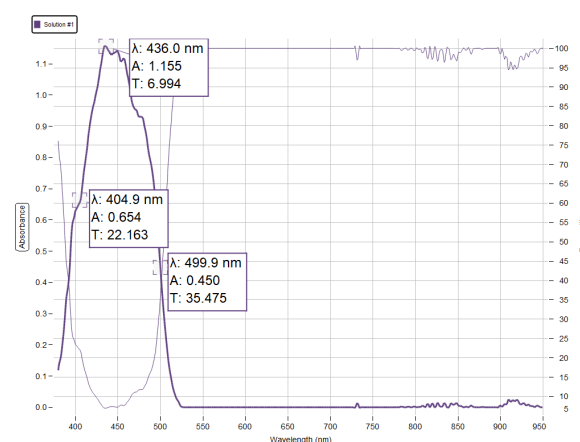


Figure 6: Absorption graph of the yellow dye cuvette

An absorption edge was identified at  $732 \pm 3$  nm. According to Sutherland, photovoltaic semiconductors' ideal band gap energy is between 1 and 1.8 eV [2]. Using the conversion equation,  $E(\lambda) = 1240/\lambda$ , the band gap energy of that absorption edge is  $1.7 \pm 0.01$  eV; this puts the yellow dye's band gap energy within the ideal range for a photovoltaic semiconductor, which indicates it may have photovoltaic properties necessary for its use as a photovoltaic semiconductor [1].

## 4 Discussion and Conclusion

In this experiment, the light emitted by various elements was studied, and the absorbance of several dye variants was recorded. Tubes of Mercury, Hydrogen, Helium and an initial unidentified gas were excited to induce light emission. This process determined that the spectrometer used recorded wavelengths of light 19.8 nm longer than in reality through the use of Mercury. Further, a similar procedure conducted on Hydrogen exposed additional errors in the setup. Peak wavelengths in the violet and blue spectrum deviated farther from their experimental wavelengths than those in the red spectrum, suggesting that there may be a linear lengthening of wavelengths dependent on their shortness, which would constitute a distinct effect from the constant lengthening for which was previously accounted. The hydrogen-like gas equations, Equations (2) and (3), turned out to be inapplicable for calculating the emission energy and peak wavelength of helium atoms, as the repulsive force between the two electrons in helium atoms affects the energy state. When the unknown gas was excited, its spectral profile most closely resembled that of Krypton. The transmittance and absorbance of the colored dyes follow the relationship  $A = -\log_{10}(T)$  and the peak wavelength for each color demonstrates that each dye absorbs light at specific wavelengths: 606.4 nm for blue, 436.9 nm for red, and 433.2 nm for green.. Finally, the yellow dye was examined, and an absorption edge with a band gap energy of 1.7 eV was found, which is within the ideal range for substances with potential photovoltaic properties. Two major sources of error may have had non-negligible effects on the data collection for which adjustments were not made at the time. First, the experiment was conducted in a well-lit room with windows and lights, exposing the probe to extra light not generated by the excited gas. In addition, the glass tubing separated the probe from the gas, which may have also affected the light. Secondly, when the cuvettes were being studied, the spectrometer produced three variants of light: white, violet and blue. While the cuvettes had rigged sides to prevent light leakage, some light may have been included in the unintentional measurements. In conclusion, the light emitted from excited gasses can be used to determine the unique traits of the gasses and the absorption of substances can also be used to predict their

properties.

## References

- [1] N. Krasnopskaia 2019. *Quantum States and Spectra of Gases*. [https://www.physics.utoronto.ca/~phy224\\_324/LabManuals/OLD\\_Spectrometry.pdf](https://www.physics.utoronto.ca/~phy224_324/LabManuals/OLD_Spectrometry.pdf).
- [2] Brandon R. Sutherland 2020. *Solar Materials Find Their Band Gap*. Cell Press.