MoS_2 Bandgap and Photoluminescence

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Introduction

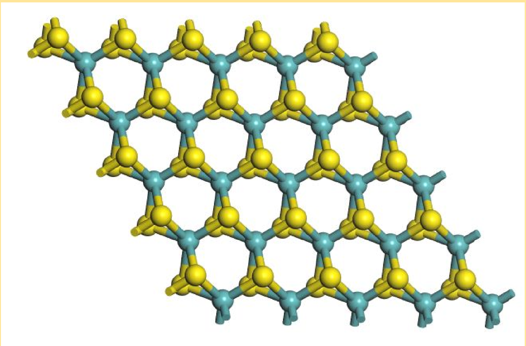
Molybdenum disulfide (MoS_2) in its chunk form functions as a semiconductor with an indirect bandgap. The characteristics of this material have been explored and its practicality has been discovered. Due to the indirect bandgap of chunk MoS_2, its electrical uses are limited and exhibits weak optical properties. As a result, it is commonly used as a simple dry lubricant or catalyst and has very little application in electrical engineering.

However, with the discovery of graphene's structure, a single layer of carbon atoms, scientists began to show interest in creating and examining different types of monolayer materials and fullerenes. When reduced to a monolayer sheet, MoS_2 becomes a semiconductor with a direct bandgap. This expands the practicality of MoS_2 in electrical components. A direct bandgap allows for greater photoluminescence and improved electrical conductivity, making MoS_2 an effective material in sensitive photodetectors and other optoelectrical devices. Controlling and studying the bandgap of MoS_2 at different levels of thickness could provide more future applications for the material in upcoming technology.

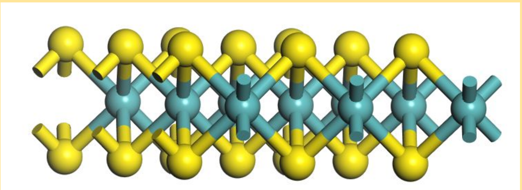
The research conducted aimed to find trends within the bandgap and photoluminescence of MoS_2 at different levels of thickness. Monolayer, bilayer, and trilayer MoS_2, along with natural bilayer and folded bilayer MoS_2 were tested and compared in order to observe changes in bandgap and peak intensity of light emitted.

Crystal of Monolayer MoS_2

Top View



Side View



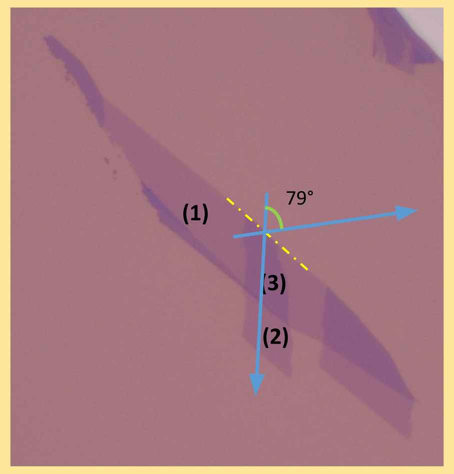
Yellow: Sulfur
Blue: Molybdenum

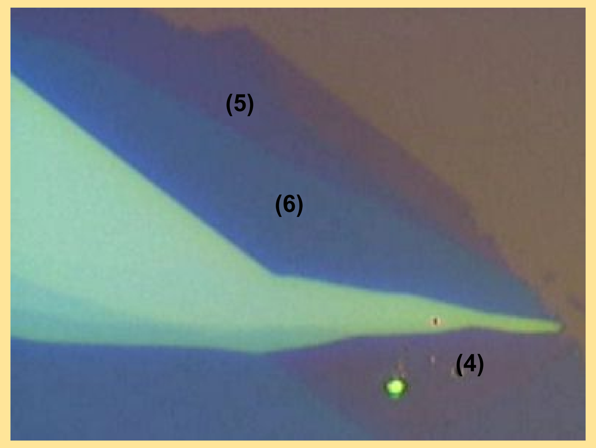
Objectives & Impact of Professor's Research

MoS_2 was tested using Raman Spectroscopy, and the resulting photoluminescence was recorded as data. The data were studied in order to find trends within the bandgap at monolayer, folded bilayer, natural bilayer, and trilayer thickness.

The results indicated that the monolayer, unfolded MoS_2 had the greatest photoluminescence when induced with energy from an external source of photons (figure 1.1). Compared to natural monolayer MoS_2, folded monolayer MoS_2 had a minor decrease in peak intensity. This is a result of the bend angle that reduces the amount of energy absorbed by the incident photons. However, the bandgap remained relatively unchanged from that of monolayer unfolded MoS_2.

The converse of this phenomenon occurred with the natural and folded bilayer MoS_2. Folded bilayer MoS_2 emitted a greater intensity of photoluminescence compared to natural bilayer photoluminescence (figure 1.2). The predicted explanation suggests that folded bilayer MoS_2 consists of two monolayers: one that is angled and one that remains flat. This combination of two monolayers emits a greater intensity than a natural bilayer, which has increased thickness. As for bandgap, folded bilayer MoS_2 has a larger bandgap than natural bilayer MoS_2. This supports the previous theory that natural bilayer MoS_2 has a greater thickness, reducing its photoluminescence.





(1) MoS_2 Monolayer
(2) MoS_2 Folded Monolayer
(3) MoS_2 Folded Bilayer
(4) MoS_2 Natural Bilayer
(5) MoS_2 Trilayer
(6) MoS_2 Few Layers

As predicted, the triple and few layer MoS_2 displayed significantly lower photoluminescence compared to monolayer. For bandgap, the minimal energy required to invoke peak intensity of light emitted from the MoS_2 decreases with the addition of each layer (figure 1.3). Decreasing energy requirements as well as decreasing photoluminescence as a result of MoS_2 thickness supports the conclusion made by Dr. Splendiani's team in *Emerging Photoluminescence in Monolayer MoS_2*- photoluminescence is only attainable at ultrathin levels. The observed trend in intensity and energy indicates that the unique property of photoluminescence is declining, and that at macroscopic scale, chunk MoS_2 would emit light at negligible intensity, regardless of the quantity of electron volts provided.

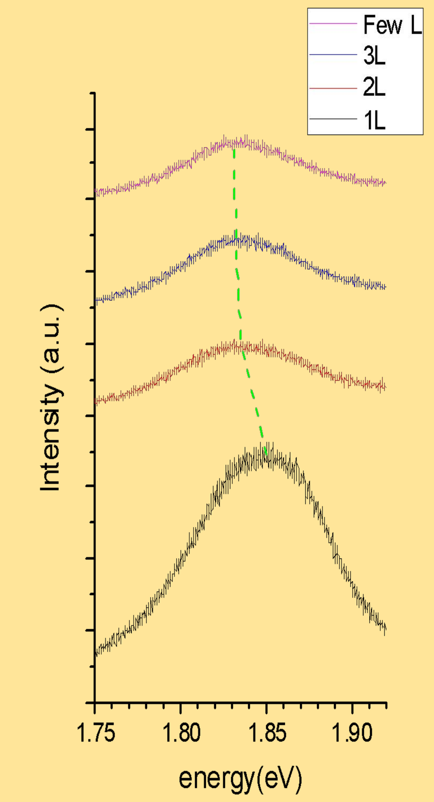


Figure 1.3
(Graphs rearranged to show bandgap trend)

Studying trends within the bandgap of MoS_2 at different levels of thickness may expand the potential application of ultrathin MoS_2 in technology. For example, advanced and well controlled optoelectronics would benefit from having a material with a direct bandgap. Using any patterns found, an optimal level of thickness could be determined which would optimize the efficiency and accuracy of optoelectronics. Photovoltaic cells also rely on having a direct bandgap material in order to transform as much solar energy into electrical energy as possible. Ultrathin MoS_2 is also a key material in memristors, which are relatively new and still require heavy research to improve. Increasing our knowledge of this material could benefit modern technology greatly.

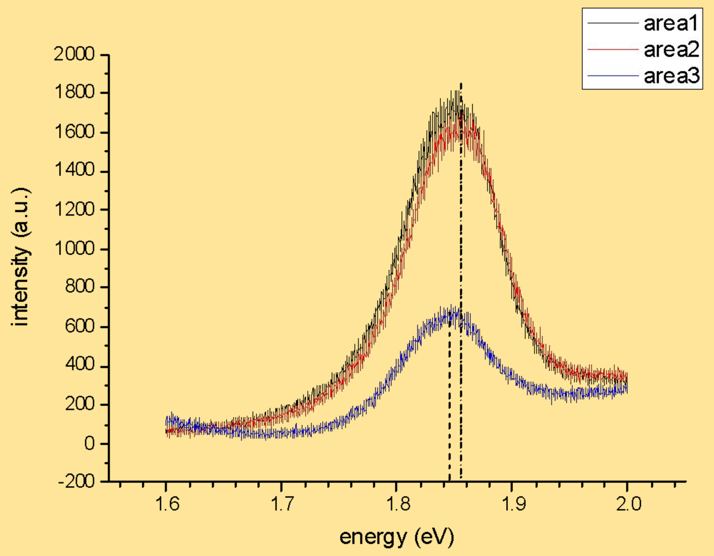


Figure 1.1

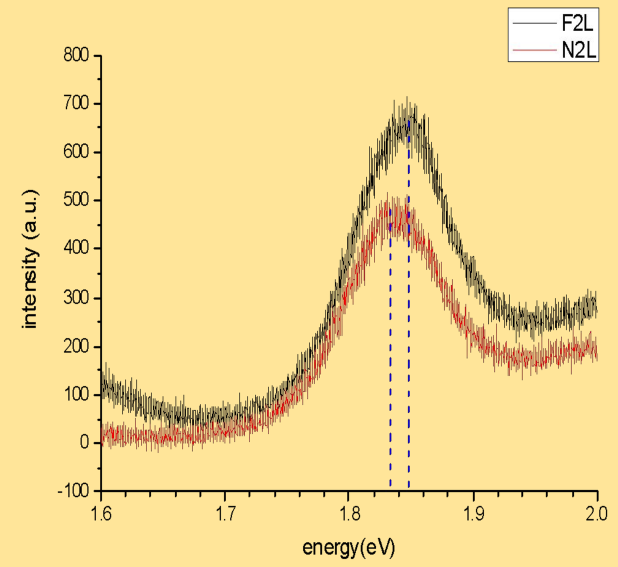


Figure 1.2

Skills Used

Throughout the research process, many skills were required:

- A strong background in chemistry was required to understand the concept of photoluminescence. For example, the ability for a material to release its own light emission after being excited by an external source of energy, such as photons, was explained by using the Bohr Model's quantized energy levels of electrons. This also helped to explain the definition of a bandgap, which is the energy gap between the covalent and valence energy levels in an atom.

- We used our understanding of standing waves and energy at quantum levels from physics in order to conceptualize the difference between direct and indirect bandgaps. Direct bandgap materials can emit light with the same energy as it absorbed from the incident light source, while indirect bandgap materials need a change in density in order to emit light. We also derived the direct proportionality between the energy of the incident photons and the wavelength of the photoluminescence using our knowledge of physics. This relation was used in our conclusion and helped to explain the trends observed in our research.

How This Relates to My STEM Coursework

Our study on the photoluminescence and bandgap of ultrathin MoS_2 applied many of the STEM standards:

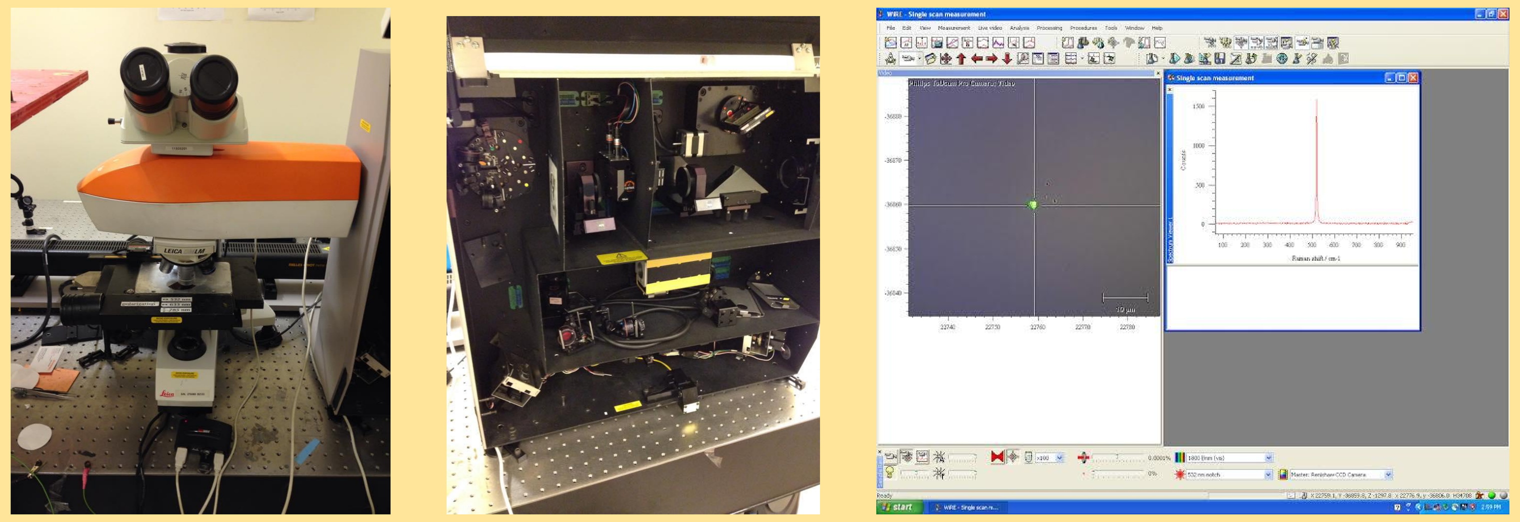
Science, specifically in physics and chemistry, was applied in the conceptualization of the basic principles behind the research. As explained in the previous section, a combination of chemistry and wave physics explained the phenomenon of photoluminescence in direct and indirect bandgap materials. These two subjects also played a role in the proposed explanation of the effect observed in our experiments. As a result, we successfully determined conclusions about the relation between a material's thickness and emitted light intensity.

Advanced lab equipment and technology were used to collect data that would be impossible for humans to gather manually. Learning how to operate technology in a lab is an essential component of the STEM curriculum, and in our research, we used a Renishaw Raman Microscope along with its accompanying WiRE software to collect all of our data (figure 1.4).

Our study focused mainly on electrical engineering. By learning more about the photoluminescence of MoS_2, we aimed to expand the opportunities to create smaller, more efficient, and more complex electrical components. Optoelectronics, such as sensitive photodetectors and variable transistors, will benefit greatly by having a new material to add to their complexity.

Mathematics was applied in order to calculate and measure the results from the Raman Spectroscopy. However, in this situation, most of the calculations were performed by the WiRE software. The results were compiled into graphs that were used in order to accomplish our goal.

Figure 1.4



A Raman Microscope and the WiRE software compiling the data for a sample of silicon

Future Plans and Advice

This research has given me a greater understanding of the work involved in actual college research and the information involved in the field of electrical engineering and 2D materials. As a result, I plan to apply to a multitude of colleges in computer or electrical engineering to gradually expand my knowledge. In the distant future, I hope to one day be able to conduct my own research at a university, similar to my own experiences at USC.

This summer internship was a great experience for me and my fellow peers. Although most of the information was sophisticated and advanced, it was beneficial and helped me decide what field I wanted to study. The program provided many resources and connections that taught me more about the subject of my research, improving my understanding of physics and chemistry. It also introduced me to technology that I had previously been unaware of, giving me experience using advanced lab equipment that a high school can not provide.

Acknowledgements

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