Alexandra Ly

Chemistry

Thesis

Abstract

My project was on the design, modelling, and synthesis of a BODIHY (boron difluoride hydrazone) dimer. In previous studies, BODIHY dyes were synthesized with significant fluorescence in solid-state but not solution state. It was found that in solid state, the dimer fluoresced due to aggregate-induced emission (AIE), meaning that the structure of the molecule was restricted in solid state and had no choice but to release energy through emission. In solution, however, as the molecules can be freely floating without interference of other molecules around, the energy was released through the freely-rotating substituents on the dye. Thus, my project aimed to design a molecule using computational chemistry methods that could possible emit light in solid state using AIE and also in solution by a restricted dimer structure and minimal substituents. After fully studying and investigating the optoelectronic properties of the molecule computational, the goal was to also synthesize the molecule and compare the results to the computational found results.

How enjoyable was using an integrated approach?

I would have never thought to investigate a molecule with computational methods. Given that the project itself would have been a failure without any additional computational results, it showed that there was more to talk about rather than just the synthesis of a molecule and there are more ways than just analyzing an already made molecule when performing synthetic chemistry.

Were there any difficulties integrating sciences?

Definitely! I had to learn a whole new sub-discipline of chemistry that was heavily involved with math and computer sciences, which I have zero to no knowledge of. It was hard to understand the language and look at my discipline in a completely new way.

Any advice for future students?

Do your research before choosing your professor. Specifically for chemistry, there is a chance you will get your second or third choice. If that is the case, choose very popular options for your second or third choice so your number one choice is more likely.