Development of a Computational Method for Rapid Identification of Organic Molecules for Efficient Solar Energy Conversion

Bhatnagar, Anshul

Solar cells are traditionally made of silicon, which is expensive to fabricate. Organic molecules are much cheaper to fabricate but are also less efficient than silicon in converting solar energy into electrical energy. Researchers are thus searching for organic molecules with high conversion efficiencies. The current process of molecule discovery is very time-consuming as there are millions of organic molecules. Each molecule needs to be first painstakingly synthesized in a lab and then synthetically tested for its conversion efficiency. The research idea is to create a new method to speed up this process by reversing these steps. In this novel method, computational chemistry is used to first find the conversion efficiency of a molecule and only if it is high enough, synthesize it in a lab. One can thus avoid synthesizing molecules that will ultimately have low efficiencies. This method was demonstrated on 18 organic triptycene molecules but can be used for any molecular scaffold. Triptycene was chosen because it can rapidly self-assemble itself into well-organized supramolecular architecture, which maximizes intermolecular charge transfer efficiency. Computational chemistry was used to determine how to connect the chromophores of each of the 18 triptycene molecules to the core to maximize intramolecular charge transfer efficiency. Next, beta values were computed for each of the 18 triptycene molecules, as molecules with the highest beta values are predicted to have the highest conversion efficiencies when used in solar cells. The method was validated on previously synthesized and tested triptycene molecules. This model correctly predicted the order of their efficiencies, thus verifying this faster and cheaper method for identifying molecules for solar cell use.