Utilizing Molecular Dynamics Simulations of Crystalline Poly(3-hexylthiophene) to Study Water Diffusion

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Many experts agree that energy may become the most important issue that society will face in the future. As fossil fuel sources are quickly being depleted and nuclear energy has proven to be largely dangerous, renewable energy is quite possibly the best method to further research for future energy production. Solar panels are growing in popularity as scientists continue to research alternatives to current means of energy production. But one of the biggest problems society faces is the availability of these options – primarily solar energy. Silicon solar panels, while very reliable, have a great deal of limitations in that they are brittle, expensive, and difficult to manufacture. However, a polymer alternative to silicon solar cells called poly(3-hexylthiophene) [“P3HT”] is undergoing great amounts of research. This organic, cheap, and easily-produced solar cell is a great advance in the scientific community, but it comes with problems of its own – namely that water very easily causes degradation. This project’s primary goal is to run molecular dynamics simulations to study how water molecules move throughout the structure of P3HT and degrade the molecule. The initial prediction was that the presence of more water molecules would lead to further degradation. By running various simulations with increasing amounts of water molecules in the P3HT structure, the diffusion of the water was monitored and led to the general conclusion that as water concentration increased, predicted degradation increased. These results largely support the hypothesis.

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