A Computational Approach to Photo Oxidized Degradation Process of PTB7 Polymer

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As power conversion efficiencies(PCE) of organic photovoltages(OPVs) are over 10%, now the life time of the device is become a crucial point to overcome for commercialization. In order to increase the durability, we need to prevent degradation of the polymer. But unfortunately degradation mechanism of photovoltaic materials has rarely been investigated. In this work, we investigated PTB7 polymer, which is widely used in OPVs, by FT-IR spectrum and DFT calculations. First, we record IR spectrum of PTB7 increasing the illumination time of solar simulator. Then, we use DFT calculation to get vibrational frequencies of the proposed intermediates. To trace a photochemical degradation mechanism, we compared the experimental and the computational IR value. We found the candidates of which experimental IR spectrums are well matched with DFT calculation. Our findings provide clues where the molecule breaks and ways to make stable OPVs by modifying molecule.

References

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