A Raman Spectroscopic Approach to Photo-Degradation Process of PTB7-Th Polymer

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Abstract

Organic photovoltaics composed of conducting copolymer and fullerenes have many advantages compare to silicon based solar cell such as low-cost, light-weight, solubility, flexibility etc. Moreover, with consistent efforts, power conversion efficiency of OPVs comes up to 12%, OPV shows promising potential to commercialization. However, the degradation is an obstacle to use OPV in daily basis. The conducting polymer easily goes degradation process in ambient condition with O_2 and results in sunlight absorption decrease which drops the device performance. In this work, to see the difference between pristine PTB7-Th and degraded one in molecular level, we use home-built Raman spectroscopy with visible pules for degradation. Combined with the DFT calculation, the emerging peak after degradation could be assigned to the formation of hydroxyl group (-OH) on the thiophene ring in the side chain. We hope that this report could be the clue to find the function of the side chain thiophene during photo-degradation process.

Introduction

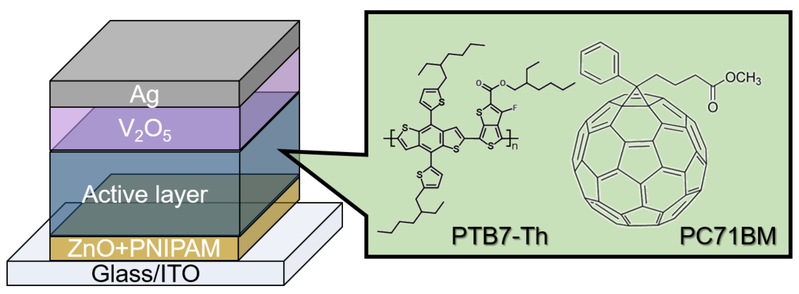

Figure 1. Device structure and Active layer component

PTB7-Th is known as a more improved solar cell donor than PTB7 because of the coplanarity of backbone and the red shift of the absorption spectrum. In our research, we could find the clue that during oxidation, the reaction takes place on the thiophene ring in the side chain. This reaction reduces the oxidation of the backbone, which initiates the overall degradation.

Raman setup

When we use commercial Raman spectroscopy, there are some limits to customize. Especially objective lens bring us spatial limits. To overcome this problem, we set up the Raman spectroscopy using parabolic mirror to measure the molecular vibration modes during operating the solar cell. The scheme of home built set up is shown below.

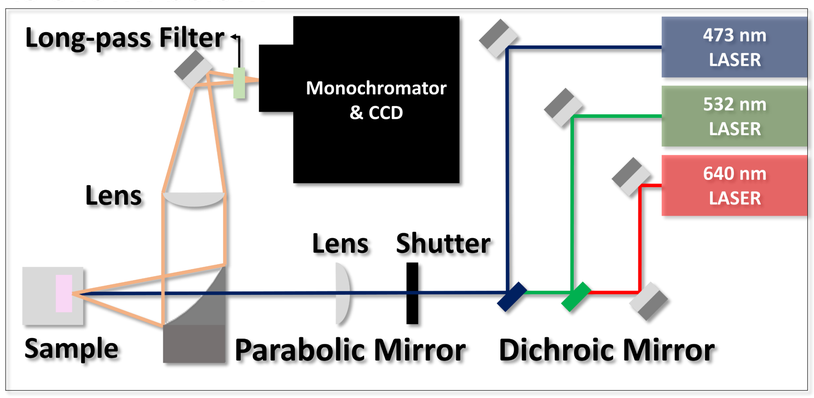

Figure 2. The scheme of Home-built Backscattering Raman Spectroscopy

Results

Photo degradation of PTB7-Th – Experimental result and calculation data

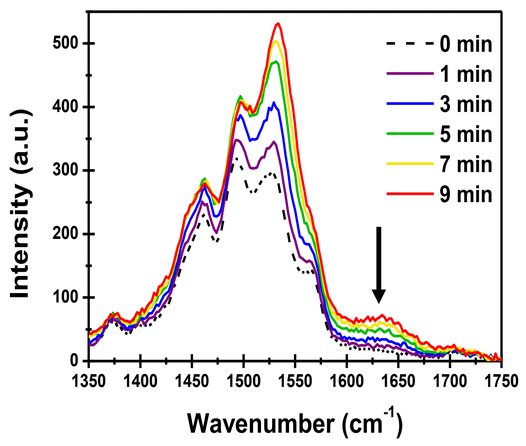

Figure 3. Raman spectra of PTB7-Th film during degradation under ambient condition

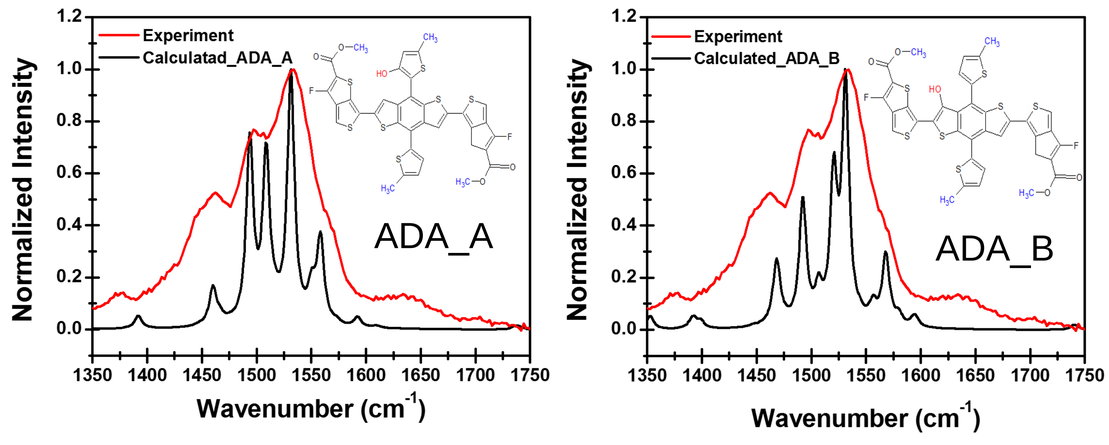

Figure 4. The comparison of Experimental data(Red) and calculation data(Black)

Comparison of the Raman spectra intensity of the calculation data – Side chain dependence

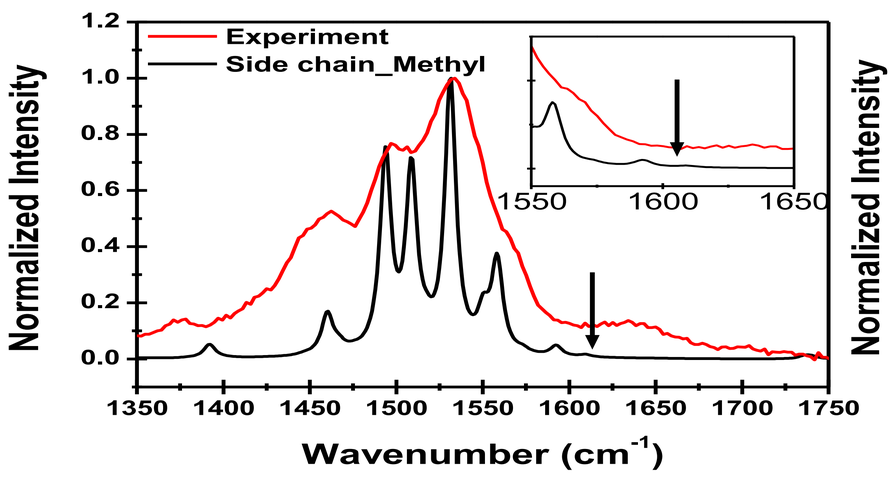

Figure 5. The comparison of experimental data and calculation data of ADA-form methyl side chain

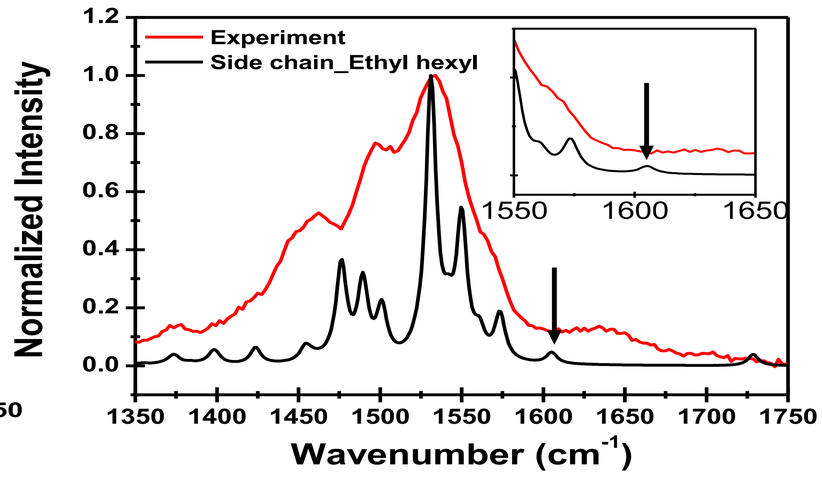

Figure 6. The comparison of experimental data and calculation data of monomer-form ethyl hexyl side chain

Initial oxidation process

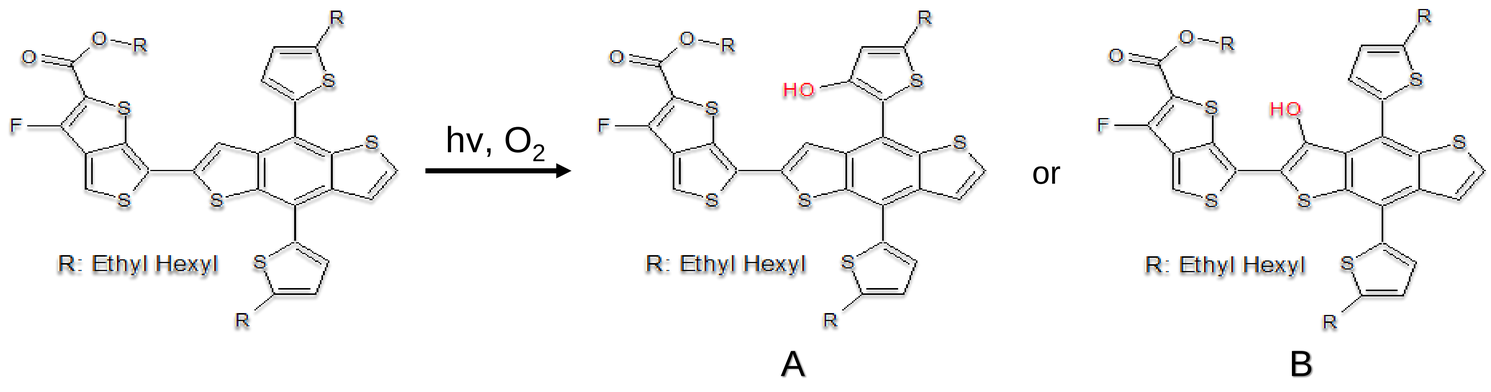

Figure 7. The scheme of initial oxidation process

Computational details

The computations of PTB7-Th oligomer(ADA), and PTB7-Th monomer reported in this work were carried out using **Gaussian 09** program package. All structures were optimized & calculated frequency in gas phase using the **density functional theory(DFT)** method with **6-31G(d, p)** basis level with the alkyl chains in the side chain reduced to methyl groups except for the PTB7-Th monomer which conserves the side chain components. Peak positions are scaled by 0.975.

Conclusion

In this research, the photo-degradation of PTB7-Th in ambient condition takes place. By using the DFT calculation, we could assign the unique peak at 1630 $cm^{-1}$is due to the hydroxylation of the thiophene ring in side chain. We hope that this report would be helpful to understand the photo-degradation mechanism of PTB7-Th polymer.

Reference

1. Razzell-Hollis J, Wade J, Tsoi WC, Soon Y, Durrant J, Kim JS. Photochemical stability of high efficiency PTB7: PC 70 BM solar cell blends. Journal of Materials Chemistry A. 2014;2(47):20189-95.

Acknowledgment

This work was supported by the Institute for Basic Science IBS-R023-D1