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

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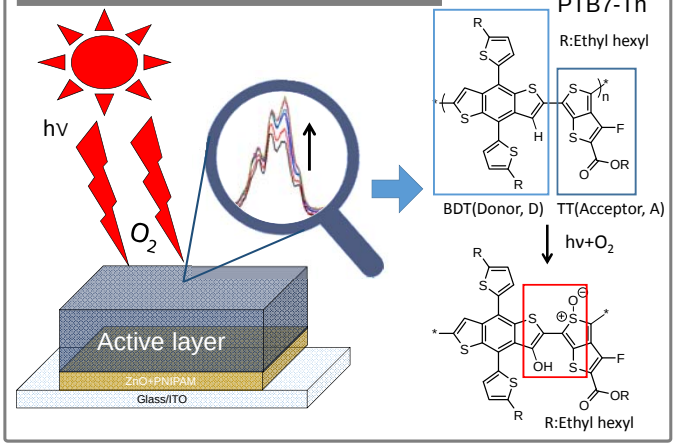
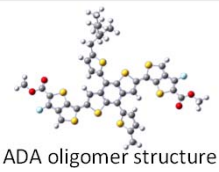
Abstract

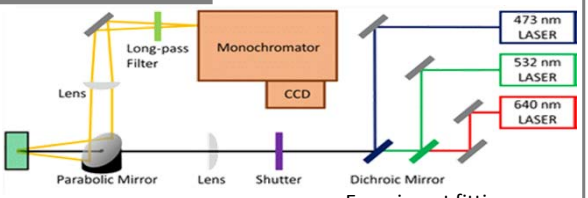
Organic photovoltaic(OPV) is one of the most promising chemical components due to its potential to becoming next generation solar cell such as low cost, flexibility etc. Because of its potential, OPV has been studied to improve the power conversion efficiency. However, there is the Achilles heel of OPV, photodegradation. In the ambient condition, the stability of OPV is much lower than silicon based solar cell. In this research, we use our home-built Raman spectroscopy to observe the photodegradation process of PTB7-Th in molecular level. Combined with DFT calculation and paper research, we could find the plausible degradation product. The generation of hydroxyl group in BDT unit and S=O bond in TT unit results in the change of Raman spectrum. We hope this research would be the clue to find other OPV degradation mechanism.

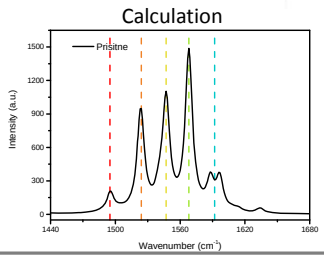
Introduction



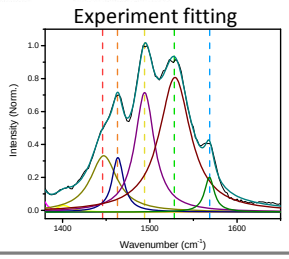
Calculation & Raman setup





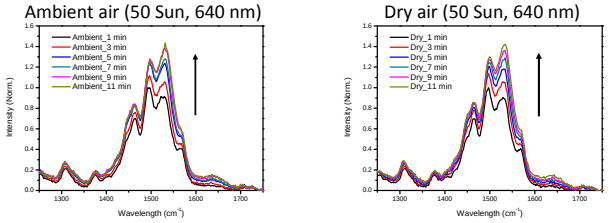


- Peak assignment
  - BDT+TT(Backbone)
  - BDT
  - BDT+TT
  - BDT
  - BDT+TT

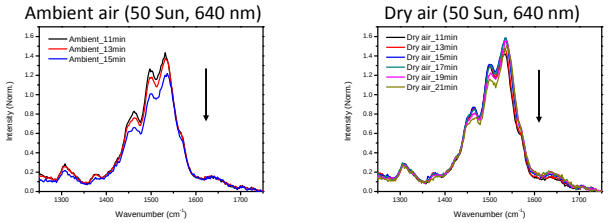


Results

- The main component that affect the initial degradation

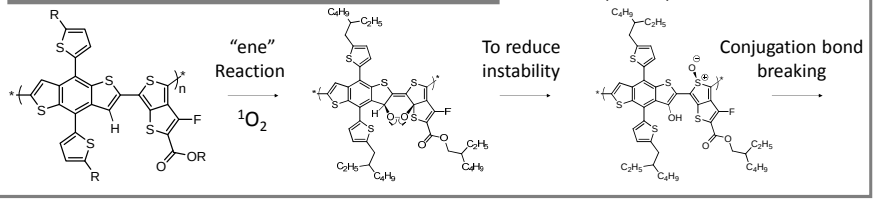


There is no difference between ambient and dry air condition
→ Oxygen is the main factor in initial degradation

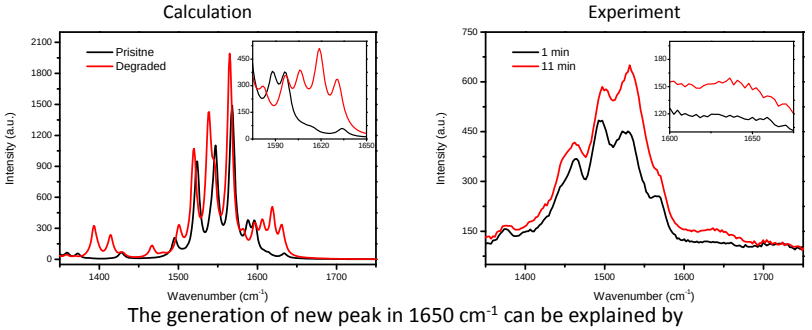


After initial degradation, decreasing rate is different.
→Water may affect the degradation after initial degradation

Predicted mechanism



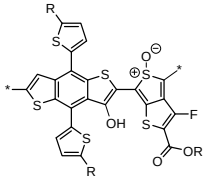
Calculation vs Experiment



The generation of new peak in 1650 cm^{-1} can be explained by the calculation Raman spectrum of the expected product

Conclusion

- In initial degradation process, oxygen is the major factor.
- Through ene reaction, the degradation product is generated.



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Acknowledgment

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