

# Studying the Affect of Substituted Side Groups for Various Fullerene Derivatives and its Importance to OPV Devices

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## Abstract

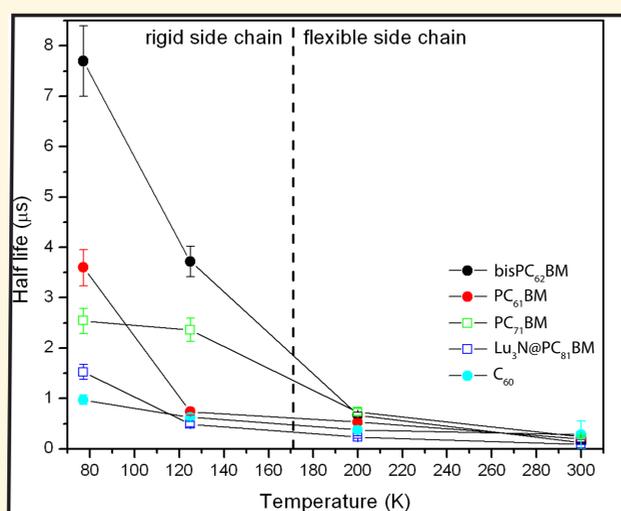
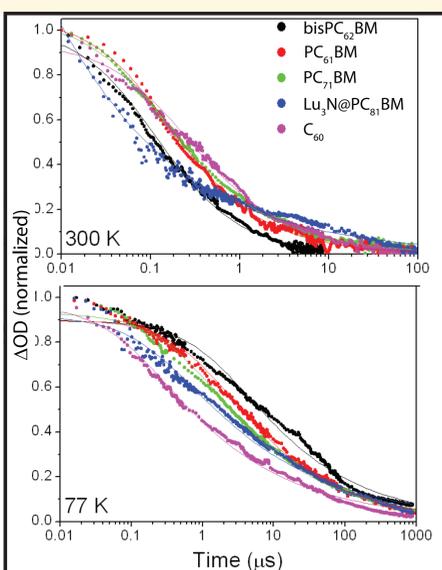
Fullerene derivatives are frequently used as electron acceptors in organic photovoltaic (OPV) devices due to their high electron affinities, high electron mobilities, and their favorable morphological interactions with many OPV polymers. These fullerene derivatives have substituted side groups to make them soluble in organic solvents used during OPV fabrication. The presence of these side groups also change the electronic properties, mobilities, recombination kinetics, and morphology, and hence the OPV characteristics of the devices.

We performed ultra-fast laser spectroscopy measurements to study the recombination kinetics within a polymer:fullerene system and found that the electrically inactive side groups serve as blockers that hinder charge recombination. We have also used differential pulse voltammetry (DPV) to study the reduction states for various fullerene derivatives and have found that a high amount of impurities are present in the samples. This result is also supported by high-performance liquid chromatography (HPLC) measurements. Scanning Transmission Electron Microscopy (STEM) was also used to image the morphology of bulk-heterojunctions (BHJ) with different fullerenes.

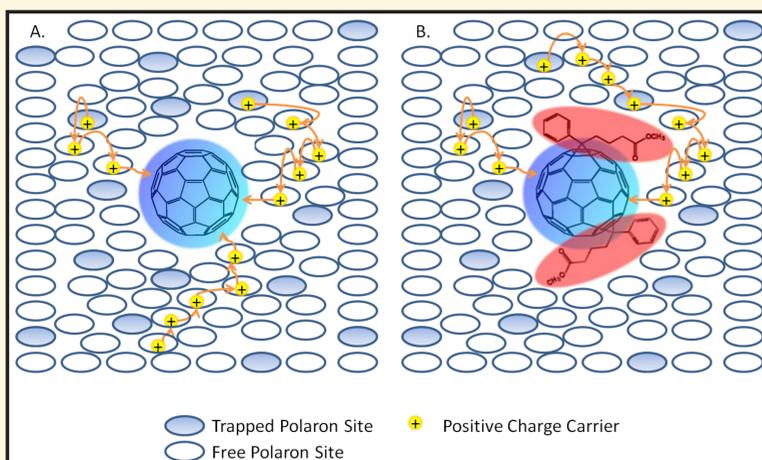
This work has given us better insight to the function of fullerene side groups and their effect on OPV operation. Having a better understanding of the effect of these side groups will help us further understand OPV device physics and will also assist in the design and development of new fullerene derivatives that will help further improve OPV device efficacies.

## Temperature-Dependent Nanosecond Transient Absorption Spectroscopy

Recombination in poly-3-hexylthiophene (P3HT) blends with five fullerene acceptors was resolved with temperature-dependent transient absorption spectroscopy. Recombination rates were temperature and acceptor dependent with differing timescales originating from acceptor functionalization and fullerene size.

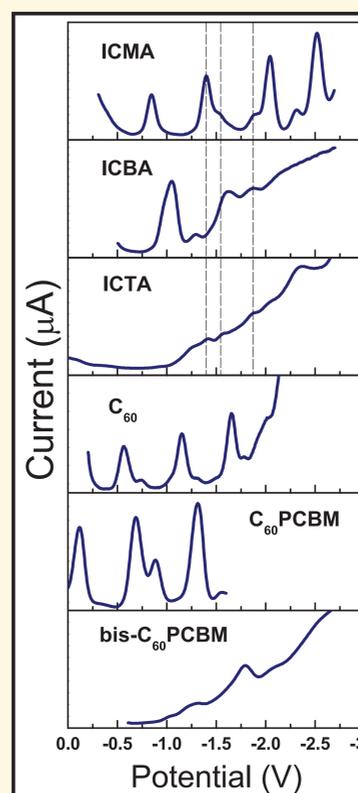
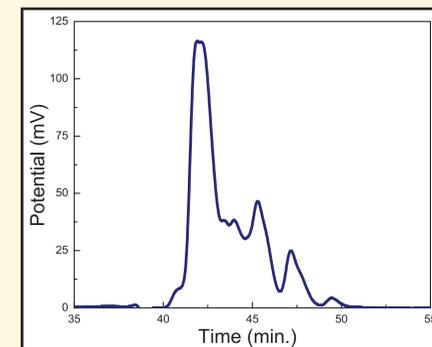
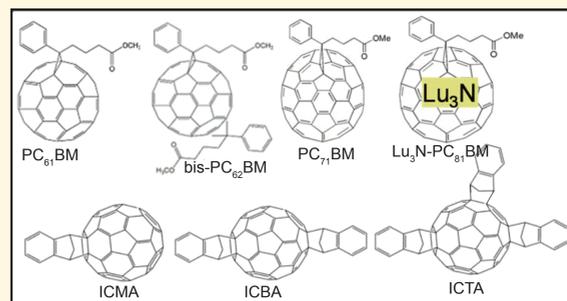


The temperature and acceptor-dependent half-lives for the recombination. Acceptors with increasing numbers of sidechains (bis > mono > C60) or decreasing fullerene size (C60 < C70 < C80) exhibit slower recombination kinetics in P3HT:fullerene thin films at low temperatures.



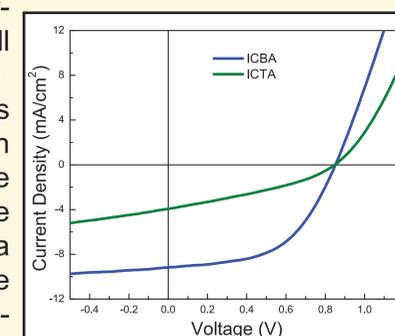
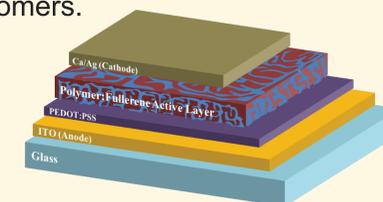
The recombination kinetics was correlated to average distance between the fullerene cage and donor site with functionalized moieties acting as dielectric shields to hinder recombination. The polaron must hop to a site near the fullerene cage before recombination can occur.

## Analytical Chemistry of PCBM- and Indene-Substituted Fullerene Samples



DPV (left) and HPLC (top right) measurements show a high impurity content for the various fullerene samples. The impurities are observed on the DPV plots by the presence of small peaks and shoulders between the main reduction peaks. The HPLC plot for ICTA shows that there are about 10 different components in the sample. These impurities are most likely other fullerene derivatives and isomers.

The IV curves (right) show a significant difference in performance between ICBA and ICTA devices. The ICTA device suffers from very low fill factor and low short-circuit current. This low performance can be due to poor charge transport from the presence of the extra indene group or the high impurity concentration of the sample.



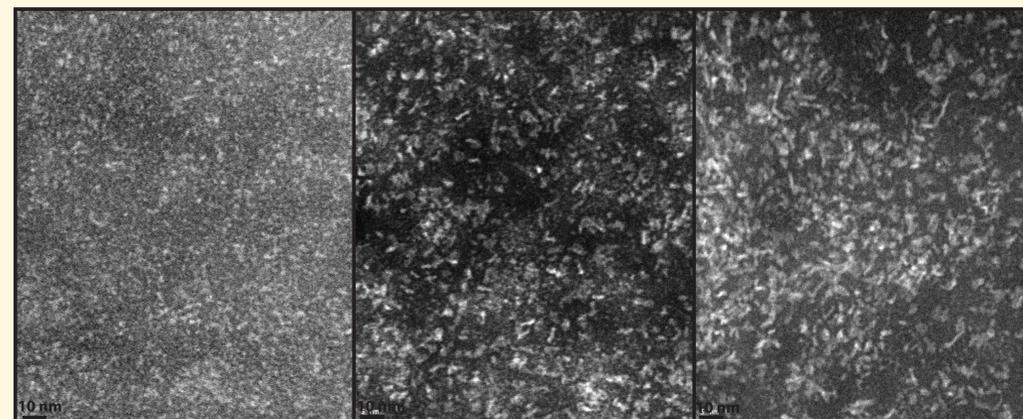
## Side Group Dependence on Morphology

Scanning Transmission Electron Microscopy (STEM) images of bulk-heterojunctions consisting of 1:1 wt. ratio of P3HT and indene fullerenes. The samples were cast from chlorobenzene and annealed at 180 °C. It is shown that the number of side groups present on the fullerene affects fullerene aggregation. Increasing the number of indene side-groups causes larger and more branched fullerene aggregates.

ICMA

ICBA

ICTA



## Acknowledgement

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## References

(1) Busby, E.; Rochester, C. W.; Moulé, A. J.; Larsen, D. S. Chemical Physics Letters 2011, 513, 77.