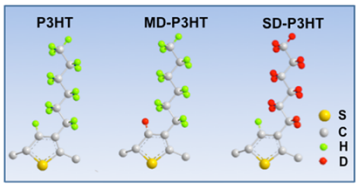
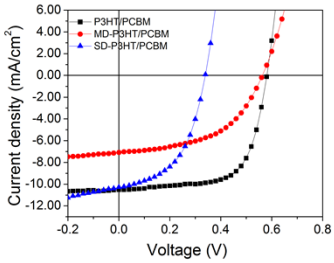
Isotopic effects of deuteration on the optoelectronic properties of conducting polymers





Top: Chemical structure of P3HT, and its main-chain (MD P3HT) and side-chain (SD-P3HT) deuterated isotopes.
Bottom: Distinctly different J-V characteristics of the three P3HT isotopes in $PC_{60}BM$ blend photovoltaics.

Work was performed at the Center for Nanophase Materials Sciences, ORNL

Scientific Achievement

We show that selective substitutions of deuterium (D) on the backbone or side-chains of conducting polymer poly(3-hexylthiophene)s (P3HT) significantly change their optoelectronic response in P3HT/PCBM ([6,6]-phenyl-C61-butyric acid methyl ester) photovoltaics.

Significance and Impact

Our work shows that isotopic substitution, once thought to be a benign modification, provides a new means to tune the optoelectronic properties of conducting polymers used for solar cells by affecting their intra- and inter-polymer chain interactions.

Research Details

- Developed a series of P3HT isotopes by selectively substituting deuterium on the backbone (MD-P3HT) or alkyl group (SD-P3HT).
- Integrated approaches including neutron/x-ray scattering, TEM and theoretical modeling to understand the origins of the large effects of D on the optoelectronic and structural properties.

M. Shao, J. Keum, J. Chen, Y. He, W. Chen, J. F. Browning, J. Jakowski, B. G. Sumpter, I. N. Ivanov, Y.-Z. Ma, C. M. Roulea, S. C. Smith, D. B. Geohegan, K. Hong, K.Xiao, *Nature Commun*. **(2014)** DOI: 10.1038/ncomms4180.

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Highlight Narrative: We report a study of the isotopic effects of deuterium substitution on the structure, morphology, and optoelectronic properties of regioregular poly(3-hexylthiophene)s (P3HT) with an integrated approach that combines the synthesis of deuterated materials, optoelectronic properties measurements, theoretical simulation, and neutron scattering. Selective substitutions of deuterium on the backbone or side-chains of P3HT result in distinct optoelectronic responses in P3HT/[6,6]-phenyl-C61-butyric acid methyl ester (PCBM) photovoltaics. The weak non-covalent intermolecular interactions induced by the main-chain deuteration change the film crystallinity and morphology of P3HT/PCBM blends, and consequently reduce the short circuit current, while decreased electronic coupling, the formation of a charge transfer state, and increased electron-phonon coupling result from side chain deuteration and induce a remarkable reduction in open circuit voltage.

Reference:

"The isotopic effects of deuteration on optoelectronic properties of conducting polymers"

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