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Synthesis and Characterization of Soluble Thiophene-, Selenophene- and Tellurophene-Vinylene Copolymers

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Organic electronic devices based on polymers received significant attention in the last decade, especially for organic photovoltaics (OPVs) and field-effect transistors (OFETs) despite their performances and stability clearly falling short of today's state-of-the-art crystalline silicon or copper indium germanium selenide (CIGS)-based devices. Flexibility in the manufacturing, light weight, lower fabrication cost, ease of integration into various devices, and large area coating are some of the major potential advantages of polymers over inorganic devices.

1 Among organic polymers, conjugated polymers attracted widespread attention for a wide range of applications. Thiophene-containing conjugated polymers, especially, poly(3-alkylthiophne) (P3AT) has been subjected to intensive research over last decade due to their excellent optical and electronic properties.

2 Moreover, poly(thienylenevinylene) (PTV) class of polymers displays high charge carrier mobilities in OFETs and promising performances in OPVs.

3 When a single solubilizing alkyl chain is included onto the PTV backbone, the resulting copolymer can be solution processed for optical devices. One simple strategy to manipulate the copolymer property is by changing the heteroatom of the thiophene from sulfur to other chalcogens, selenium or tellurium.

4 Theoretical calculations indicated that substitution with selenium or tellurium may reduce the optical band gap of the resulting polymer in comparison to their sulfur-containing analogues. Inclusion of larger and more polarizable selenium or tellurium also expected to have a strong influence on the charge transport properties. Notably,

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Heeney and co-workers showed that the band gap of P3AT can be reduced by as much as 0.3 eV by only substituting sulfur with selenium in the polymer backbone.

5 The reduction of band gap resulted from larger and more polarizable selenium facilitate better π orbital overlap with the polymer backbone and thus stabilize the polymer LUMO (lowest unoccupied molecular orbital). Low-lying LUMO levels are believe to facilitate both electron injection and transport. Recently, PBDTT-SeDPP polymer showed a high Jsc of 16.8 mA/cm^2, a Voc of 0.69 V, and a FF of 62%, enabling the best PCE of 7.2%.

6 However, despite fascinating properties of selenium substituted polymers, tellurium containing polymers are less explored, may be due to challenging tellurium chemistry. Jahnke and co-workers recently reported first soluble tellurophene polymer, poly(3-alkyltellurophene) (P3ATe), prepared by both electrochemical and Kumuda coupling polymerization method.

7 Even though, preliminary PCE (1.1%) was modest, tellurium substitution resulted in red-shifted film absorption.In this contribution, we report the synthesis and characterization of vinylene copolymers containing 3-alkylthiophene, selenophene or tellurophene. This allows us systematically investigate the role of selenium or tellurium on the polymer properties. Here, we report the first synthesis of novel 2,5-dibrominated 3-alkyltellurophene monomer and its Pd[0]-catalyzed copolymerization with (E)1,2-bis(tributylstannyl)ethylene to afford poly(3-alkyltellurophenylenevinylene) (P3ATeV).

8 We compare the optoelectronic properties of P3ATeV with analogous sulfur (P3ATV) and selenium (P3ASV) containing polymers. Preliminary OFET data will also be incorporated. Scheme 1. Structures of P3AX, P3AXV copolymers.

References

1. Gang Li, Rui Zhu and Y. Yang, Nature Photonics 2012, 6, 153–161.
2. M. T. Dang, L. Hirsch and G. Wantz, Adv. Mater. 2011, 23, 3597–3602.
3. D. Astruc, E. Boisselier and C. Ornelas, Chem. Rev. 2010, 110, 1857–1959.
4. M. Jeffries-EL, B. M. Kobilka and B. J. Hale, Macromolecules 2014, 47, 7253–7678.
5. M. Heeney, W. Zhang, D. J. Crouch, M. L. Chabinyc, S. Gordeyev, R. Hamilton, S. J. Higgins, I. McCulloch, P. J. Skabara, D. Sparrowe and S. Tierney, Chem. Commun. 2007, 5061–5063.
6. L. Dou, W.-H. Chang, J. Gao, C.-C. Chen, J. You and Y. Yang, Adv. Mater. 2013, 25, 825–831.
7. A. A. Jahnke, B. Djukic, T. M. McCormick, E. B. Domingo, C. Hellmann, Y. Lee and D. S. Seferos, J. Am. Chem. Soc. 2013, 135, 951–954.
8. M. Al-Hashimi, Y. Han, J. Smith, H. S. Bazzi, S. Y. A. Alqaradawi, S. Watkins, T. D. Anthopoulos, M. Heeney, Chem. Sci. 2015, DOI: 10.1039/C5SC03501E.