Electronic Supporting Information

For

Parallel Design Strategy and Rational Study of Crystal Engineering of Novel 3,4-Ethylenedioxythiophene Derivatives for Solid State Polymerization

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1. DSC scans of the monomers

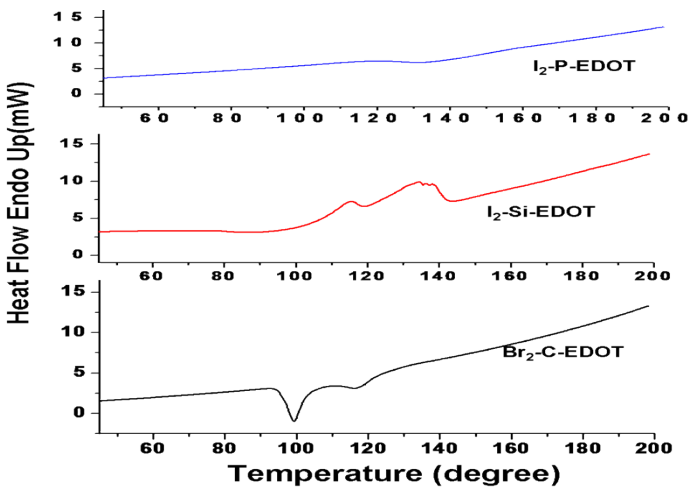

Figure S1. DSC scans of the monomers at a heating scan rate of 10 °C /min.

The DSC curves shows that these monomers melt points are over 80 °C. Meanwhile, Br_2-C-EDOT shows exothermic polymerization peaks around 98 °C and small one around 115 °C. However, I_2-P-EDOT shows weak peak around 135 °C. While in the case of I_2-Si-EDOT, it seems that it has two endothermic peak. The former peak may be related with its T_g and the second one may related to phase transformation or others.

2. In-situ XRD patterns for I_2-P-EDOT

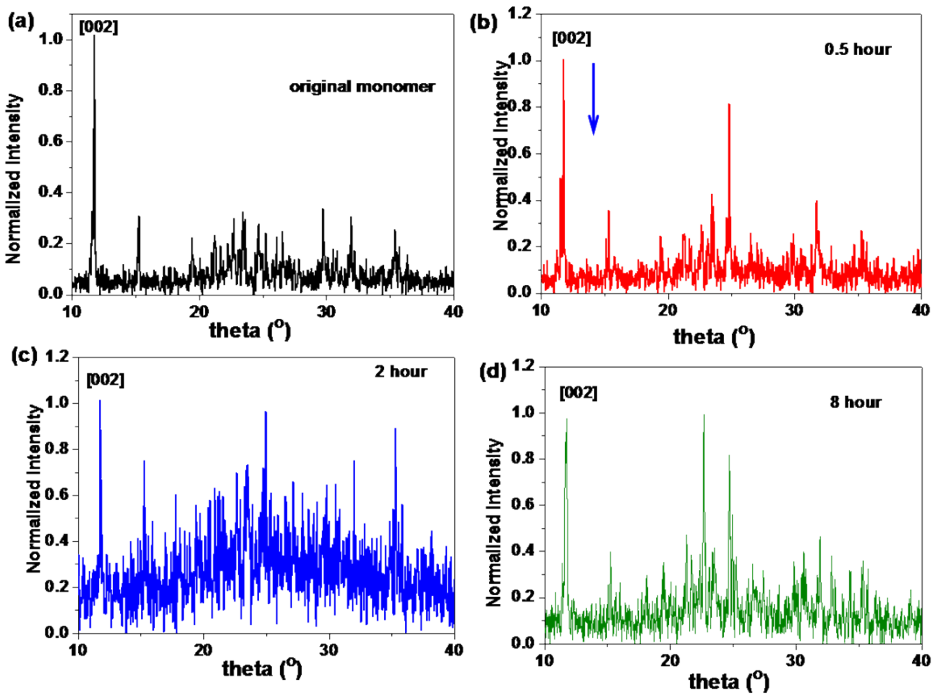

Figure S2. In-situ XRD patterns of the monomer of I_2-P-EDOT at different annealing time at 80 °C.

In order to find solid evidence of the initial polymerization procedure,

monomer of I_2-P-EDOT was selected as an example and its in-situ XRD patterns were presened in FigS2. It is obviously that drastic decrease of [002] phase intensity was observed at the initial 2 hours' polymerization, which means that the initial polymerization occurs at the ab-plane in the crystal. Therefore, such result is well consistent with our pridiction of the most possible 1st polymerization pathway along *b*-axil direction at crystal analysis.