

Abstract Submitted  
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**Exploring the correlation between molecular conformation and optoelectronic properties of conjugated polymers : side-chain versus main-chain electron acceptors**<sup>1</sup> YU-CHEN HUANG, Ph.D student , CHING-I HUANG, Professor at Institute of Polymer Science and Engineering — Polythiophene derivatives have been shown among the most promising materials for solar cell application because of their high charge mobility and light absorption. In the mostly studied, a recombination process often occurs, which is mainly due to the fact that the mobility of hole is much lower than that of electron. Hence, research about conjugated polymers containing donor-accepter pairs (such as PT-TPD) becomes quite popular because these materials have narrow band-gaps. Interestingly, these experimental studies have indicated a much more complex correlation between the optoelectronic properties and molecular conformation for polymers with acceptor units on either main or side chain. However, the effects associated with the molecular packing on the resultant chain conformation behavior and thereafter the optoelectronic properties have not been systematically discussed. In order to clarify the effects of the molecular conformation as well as the optoelectronic properties, we employ molecular dynamics and quantum mechanical methods to examine PBTPD molecules with acceptor unit (TPD) on either main or side chain

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None

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