Symp C5

# Comparison of Conformations and Electronic Structures of Poly(3,4-ethylenedioxythiophene) and Poly(3,4-ethylenedithiathiophene) in the Neutral and Doped States

# 중성 및 도웁된 상태에서의 폴리(3,4-에틸렌디옥시티오펜)과 폴리(3,4-에틸렌디티아티오펜)의 컨퍼메이션과 전자 구조의 비교

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We compared the conformations and electronic structures of poly(3,4-ethylenedioxythiophene) [PEDOT] and poly(3,4-dithiathiophene) [PEDTT] in the neutral and doped states through AM1 band calculations and modified extended Hückel band calculations. In the neutral states, PEDOT possesses a quite flat potential curve ranging from helical angles of 60 - 120°. PEDTT has a deep potential curve at the twisting angle of 90°. Due to the twisted structures, the HOMO-LUMO gaps of the neutral polymers are estimated to be larger than the gap of polythiophene. In the doped states, both polymers become planar and possess zero band gaps.