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Degradation mechanism of a low band gap polymer PTB7 by oxidation SOOHYUNG PARK, JUNKYEONG JEONG, Yonsei University, HYUNBOK LEE, Kangwon National University, YEONJIN YI, Yonsei University — Recently, the PCE of OPVs is at the 10% mark by using donor materials having a low band gap, such as poly(4,8-bis[(2-ethylhexyl)oxy]benzo[1,2-b:4,5-b']dithiophene-2,6-diyl-alt-3-fluoro-2-[(2-ethylhexyl)carbonyl]thieno[3,4-b]thiophene-4,6-diyl) (PTB7) and its analogues. In spite of the significant PCE improvement, the lifetime issue still remains open problem. To solve these technical limitations fundamentally, the degradation mechanism should be understood. It can be revealed by investigating the electronic structures of polymers with controlled exposure of oxygen, moisture and light. In this study, ultraviolet, X-ray and inverse photoelectron spectroscopy measurements were performed with step-by-step exposure of controlled oxygen, moisture and light to investigate the degradation mechanism of each polymer film. Theoretical calculations using density functional theory (DFT) were also performed to understand detailed degradation process. From the experimental results, we demonstrate that push-pull polymers are more sensitive to environmental conditions, compared with non-push-pull (conventional) polymers such as poly(3-hexylthiophene-2,5-diyl) (P3HT). In addition, we show high photo-oxidation of PTB7 is originated from the structural reason.

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