Molecular Engineering of conjugated polymer to enhance the vertical electrical properties for photovoltaic devices

Hyo Jung KIM(hyojkim@pusan.ac.kr)[1], Sangmin Chae[1], Ahra Yi[1]
Hyun Hwi Lee[2], Jiyeon Choi[3]
[1]Pusan National University, [2]Pohang Accelerator Laboratory, [3]Korea Institute of Machinery and Materials

Abstract

We report the nondestructive preparation of a polymer HTL thin film for polymer-based photovoltaics via molecular engineering with fs-laser process as well as a simple solvent process. By adopting fs-laser, we could induce face-on stacking in poly(3-hexylthiophene) (P3HT) conjugated polymer thin films. As a result, the vertical electrical charge transport enhanced about 2 times after fs-laser irradiation in comparison with pristine films. The face-on favorable stacking was related to the dipole alignment of P3HT molecules along the direction of the electric field of incoming laser. [1-3]

In case of solvent process, we found that the crystallinity and orientation of poly(3-hexylthiophene) (P3HT) molecules in the thin film were strongly dependent on the volatility of the solution, and we quantified the relationship using a combination of grazing-incidence wide-angle X-ray scattering (GIWAXS) and near-edge X-ray absorption fine structure (NEXAFS) measurements. We successfully verified the correlation between the tilt angle of the molecules and the surface energy of the films for the first time, and this result can guide subsequent research into both perovskite solar cells and organic electronics. Using our molecularly engineered films, we fabricated p–i–n-structured P3HT HTL perovskite solar cells that showed both better efficiency and greater stability than solar cells fabricated with the widely used poly(3,4-ethylenedioxythiophene) doped with polystyrene sulfonate (PEDOT:PSS) HTL. [4,5]

Keywords: *organic semiconductor, conjugated polymer, molecular engineering, GIWAXS, NEXAFS*

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