Ionization Potential Studies on Self-Assembling Perfluoroalkylated Phthalocyanine and PC61BM affected by Fluorophilic/Fluorophobic Interaction

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Discotic liquid crystalline (DLC) semiconductors are promising candidates for bulk-hetero-junction (BHJ) organic solar cells (OSCs) due to well-defined structure as forming one-dimensional pathway and the homotropic alignment. Furthermore, vertically stacked columnar structures such as hexagonal or rectangular columnar phases are very suitable and similar to ideal face-on BHJ structures for efficient OSCs. Recently, perfluoroalkylated phthalocyanines (Pcs) have been reported to give well-organized segregated nano-structure and to stabilize columnar mesophases.¹ Herein, we synthesized perfluoroalkylated or alkylated Pcs and PCBM for investigation of the effects on the fluorophobic/fluorophilic interactions in their mesophase and electronic properties. Both Pcs exhibit columnar mesomorphism and the thermal stability of LC phase is enhanced as incorporation of perfluoroalkyl group, probably due to the nano-segregation between the fluorinated and hydrocarbon moieties in the chains. In this work, ionization potentials (IPs) of the thin films of F3C7PcH₂ and F4PCBM were evaluated by photoelectron spectroscopy to give a discrepancy against the expected values on chemical structure and the origin is discussed to reveal a shield effect of perfluoroalkyl groups which surrounding the core part of discotic mesogen which play a role of charge transport when the molecules stack to form columnar structure. The difference in chemical structure for these compounds is just whether the terminal four carbons in a chain are perfluorinated or not. Fig. 1 shows IPs for spin-coated films based on perfluoroalkylated or alkylated Pc and PCBM, respectively. IP value of F4PCBM (−6.16 eV) is similar to that of PCBM (−6.25 eV). This indicates that methylene groups link the Pc and PCBM cores and perfluoroalkyl chain, indicating the far less effect of electron withdrawing character of perfluoroalkyl group on electronic structure of central core. However, incomprehensible IP values were obtained from thin-films of F3C7PcH₂ and C7PcH₂.

In this presentation, we will discuss the difference in IP values by columnar lattice arrangements, as well as notes on investigation of electrochemical properties for thin-films based on perfluoroalkylated DLCs.

Reference