Novel fullerene based materials for polymer, small molecular and multicomponent organic solar cells

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A new family of fullerene derivatives bearing chelating pyridyl appendages (PyF) was designed for the use as electron acceptors in small molecular organic solar cells comprising donor zinc phthalocyanine (ZnPc). Solution deposition of PyF on the evaporated ZnPc films yields bilayer devices where donor and acceptor counterparts are forming complexes at the diffused interphase between the layers. Such supramolecular association of the materials facilitates photoinduced charge separation and results in improved performances of the devices.

Additionally, PyF-based materials enabled fabrication of novel organic solar cell architectures that we called multicomponent. On the bottom zinc phthalocyanine layer polymer-fullerene (fullerene = PCBM+PyF) blend was deposited from the solution. Thus, multicomponent solar cells can be considered as a combination of the small molecular bilayer and polymer bulk heterojunction approaches. Charge separation in such devices occurs between ZnPc and PyF at the interface between two layers as well as in the top bulk heterojunction layer between fullerene derivatives and PCBM. As a result, multicomponent devices generate photocurrent in entire visible region (350-850 nm) with moderate efficiency (IPCE up to 40%). Encouraging power conversion efficiencies of 2.0-2.5% were achieved in the first non-optimized multicomponent solar cells.

We synthesized approximately 40 novel organic derivatives of C_{60} and C_{70} fullerenes possessing different aryl (heteroaryl) and/or alkyl groups appended to the fullerene cage trough cyclopropane moiety. It was shown that even slight variation in the molecular structures of these compounds changes significantly their solubility in organic solvents. In turn, the solubility of the fullerene derivatives affects strongly morphology of their composites with poly(3-hexylthiophene) (P3HT), used as active materials in organic solar cells. As a consequence, the solar cell parameters depend strongly on the structure and properties of the fullerene-based materials. The power conversion efficiencies for solar cells comprising new fullerene derivatives range from negligibly low (0.01%) to appreciably high (4.0%) values. The analysis of the extensive sets of data on the structure, solubility, morphology, and solar cell performance of fullerene based materials allowed us to elaborate a predictive model that might be useful in designing of superior combinations of donor and acceptor materials for efficient organic photovoltaics.