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Charge-Transfer Complexation Mechanism of Poly (4-Vinyl Pyridine)/[6,6] - Phenyl-C_{61}-Butyric Acid Methyl Ester in DMF Solution[1]

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— The mechanism of charge-transfer complexation in electron-donor(D)/electron-acceptor(A) active layer was studied for a pseudo-binary blend model system, poly(4-vinyl pyridine) /[6,6]-phenyl-C_{61}-butyric acid methyl ester in DMF. The time evolution of the system can be characterized by four distinct stages, i.e., induction, complexation, aggregation and precipitation, respectively. In the induction stage, the conformation of P4VP remained unchanged, while the UV-vis showed that the charge-transfer complexation had almost accomplished. In the complexation stage, each P4VP chains complexed with about 3 PCBM molecules at [4VP]/[PCBM]=57:1, and shrinked in size with almost no change in UV-vis spectrum. In the subsequent aggregation stage, P4VP/PCBM complexes aggregated with each other to form spherical aggregates with again unchanged UV-vis signals. FA model can be used to explain this mechanism. In the final precipitation stage, huge P4VP/PCBM agglomerate began to phase out. The almost unchanged UV-vis spectrum after the induction stage indicated that the electronic transition from ground to excited state is not necessarily to be influenced by any inter- or intra-polymer structural transition.

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