Organic semiconductors have been actively investigated to develop photovoltaic devices and light-emitting diodes (LEDs). Especially, organic solar cells (OSCs) are hoped to make economical low-priced solar energy conversion be possible. To achieve high efficiency OSCs, syntheses of new materials that have a suitable band-gap for OSCs and micro-scale morphology like a bulk heterojunction (BHJ) have been explored. OSCs based on BHJ have steadily improved, which leads to power conversion efficiencies 6–7%.

We analyze packing effects in organic donor-acceptor molecular heterojunctions from viewpoints of electronic structure calculations (Figures; (a) TFB(lowr)/F8BT(upper) complex, (b) HOMO, (c) LUMO, (d) LUMO+2) and electronic relaxation dynamics. From the first viewpoint, it is clarified that the packing structure between the donor and the acceptor strongly affects charge transfer states in which an electron transfers from the donor to the acceptor. From the second viewpoint, it is confirmed that qualitative different dynamics occurs in each different packing. These effects are caused by packing dependences of exciton binding energy, which suggest a crucial role of the exciton binding energy for molecular design of organic heterojunctions in nano-meter scale [1].

Reference