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Understanding the effects of the energy band alignment at the donor/acceptor interface on the open circuit voltage of organic photovoltaic devices

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Abstract

In organic photovoltaic (OPV) devices, the open-circuit voltage (V_{oc}) is one of the most important parameters that determines the device performance. Generally, the maximum value of V_{oc} is set by the energy gap (E_{gap}). However, the E_{gap} value of the active layer of an operating device will deviate from that based on the energy levels of the individual materials due to the occurrence of complicated interfacial physical and chemical interactions. Here, we systematically investigated the effects of the interfacial energy band alignment with different polymer donors and small-molecule acceptors. The E_{gap} values increased in the presence of an interfacial dipole, leading to a larger voltage loss (Δ) than expected.

Key words: organic photovoltaic devices, open-circuit voltage, energy gap, interfacial energy level alignment

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