Pechmann Dye Analogues Based Small Molecules as Promising Donor Candidates in Photovoltaics with Low Interfacial Charge Recombination

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The donor/acceptor interfacial charge transfer plays a crucial role in organic photovoltaic performance. The higher charge separation rate and lower charge recombination rate at the donor/acceptor interface are desirable for efficient exciton dissociation and facile charge transfer. In the present study, a series of donor-acceptor-donor (D-A-D) type small molecule donors are designed containing Pechmann dye analogues (O, S, N) which are relatively less explored in the field of organic photovoltaics. The overall photovoltaic performance and small molecule donor/$PC_{61}BM$ acceptor interfacial charge transfer are investigated using density functional theory (DFT) and time-dependent density functional theory (TD-DFT). The structural modification of the donor backbone has been performed via additional sp^2-nitrogen heteroatom incorporation in the Pechmann analogue acceptor cores. The N-heteroatom incorporation plays a significant role in lowering the charge recombination rate (K_{CR}) and increasing the charge separation rate (K_{CS}) at the small molecule donor/$PC_{61}BM$ interface. The ratio of interfacial K_{CS} and K_{CR} is found to be improved by 10^4–10^{10} times after sp^2-nitrogen substitution to the Pechmann analogue cores. Furthermore, the N-heteroatom incorporated small molecule donors are found to have enhanced open-circuit voltage. The maximum predicted power conversion efficiencies (PCEs) using the Scharber diagram could reach up to ~9% for the S-analogue of the Pechmann dye core based donor. This theoretical study is expected to provide further insight into developing high performance donor candidates using Pechmann analogues in organic photovoltaic applications.