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Research Collaboration

7. Dr. Sagar Sharma, Assistant Professor and Head, Department of Chemistry, SB Deorah College has Research Collaboration with Sridhar Sahu, Professor, Department of Chemistry, University of Alberta, Edmonton, Alberta, T6G 2G2, Canada, on studies on organic semiconductors.

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Promising small molecule Pechmann dye analogue donors with low interfacial charge recombination for photovoltaic application: A DFT study

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ABSTRACT

A series of donor–acceptor–donor (D-A-D) type small molecule (SM) donors containing Pechmann dye analogues (N, S, O) are designed and their geometrical, optoelectronic, charge transport, and photovoltaic properties are investigated using density functional theory (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 containing SM donors are found to be more air-stable due to having relatively deeper HOMO/LUMO levels than their unsubstituted counterparts. The maximum computed open-circuit voltage (V_{oc}) is 1.53 V for the N-heteroatom substituted O-Pechmann core based donor. The designed donors are expected to harvest photon energy efficiently as their simulated absorption spectra lie in the visible region (575–724 nm). 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 SM donor/$PC_{61}BM$ interface. The ratio of interfacial K_{CS} and K_{CR} is found to be improved by $10^6 - 10^{18}$ times after sp^2-nitrogen substitution in the Pechmann analogue cores. The maximum predicted power conversion efficiencies (PCEs) using the Scharber diagram reach up to ~9% for the S-analogue of the Pechmann dye core based donor. This study sheds light on promising SM donors based on Pechmann dye analogues with low interfacial charge recombination rates and high charge separation rates and also demonstrates the impact of structural modification of Pechmann dye analogue cores on air-stability and overall photovoltaic performance.

1. Introduction

The last few decades have witnessed accelerated research interest in bulk heterojunction (BHJ) organic solar cells (OSCs) comprising polymers or small molecules as light harvesting donor materials [1–6]. The maximum power conversion efficiency (PCE) for single junction solar cells based on polymer donors and fullerene acceptors recently reached over 11% [2,3]. However, polymer solar cells possess several limitations in large-scale commercial applications due to serious issues related to diverse polydispersity index, poor synthetic reproducibility, laborious purification processes, and end-group contamination. In such a scenario, small molecule (SM) donor materials provide advantages over typical polymeric counterparts. Small organic molecules have well-defined molecular weight, definite molecular structure, higher purity, tunable optoelectronic properties, and better control over batch production. Simple and minor modifications in their molecular structures have a crucial impact on organic solar cell performance, while the efficiency of polymer solar cells remains almost unaffected by such minor structural change [5–8]. For these reasons, molecular modeling and screening of effective small molecule (SM) donor materials have become active areas of interest. A tremendous effort has been devoted towards designing promising SM donor materials through structural optimization and molecular backbone modification using density functional theory (DFT) approaches without time-consuming experiments. Notably, the computational design and screening procedure contributes to databases such as the Harvard Clean Energy Project, National Renewable Energy Laboratory database for the next generation uses [9]. The most promising classes of SMs have different push–pull architectures such as donor–acceptor (D-A), D-A-D, and A-D-A [4,10–12]. The D-A-D or A-D-A architectures possess lower band gaps than the corresponding D-A systems and such modulated architectures were also reported to extend the optical absorption and enhance photovoltaic efficiency [13,14]. In comparison with A-D-A structures,

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