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Design and Synthesis of an Organic Material with High Open Circuit Voltage of 1.0 V

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Abstract : The growing need for energy by the human society and depletion of conventional energy sources demands a renewable, safe, infinite, low-cost and omnipresent energy source. One of the most suitable ways to solve the foreseeable world's energy crisis is to use the power of the sun. Photovoltaic devices are especially of wide interest as they can convert solar energy to electricity. Recently the best performing solar cells are silicon-based cells. However, silicon cells are expensive, rigid in structure and have a large timeline for the payback of cost and electricity. Organic photovoltaic cells are cheap, flexible and can be manufactured in a continuous process. Therefore, organic photovoltaic cells are an extremely favorable replacement. Organic photovoltaic cells utilize sunlight as energy and convert it into electricity through the use of conductive polymers/ small molecules to separate electrons and electron holes. A major challenge for these new organic photovoltaic cells is the efficiency, which is low compared with the traditional silicon solar cells. To overcome this challenge, usually two straightforward strategies have been considered: (1) reducing the band-gap of molecular donors to broaden the absorption range, which results in higher short circuit current density (JSC) of devices, and (2) lowering the highest occupied molecular orbital (HOMO) energy of molecular donors so as to increase the open-circuit voltage (VOC) of applications devices.8 Keeping in mind the cost of chemicals it is hard to try many materials on test basis. The best way is to find the suitable material in the bulk. For this purpose, we use computational approach to design molecules based on our organic chemistry knowledge and determine their physical and electronic properties. In this study, we did DFT calculations with different options to get high open circuit voltage and after getting suitable data from calculation we finally did synthesis of a novel D–π–A–π–D type low band-gap small molecular donor material (ZOPTAN-TPA). The Aarylene vinylene based bis(arylhalide) unit containing a cyanostilbene unit acts as a low-band- gap electron-accepting block, and is coupled with triphenylamine as electron-donating blocks groups. The motivation for choosing triphenylamine (TPA) as capped donor was attributed to its important role in stabilizing the separated hole from an exciton and thus improving the hole-transporting properties of the hole carrier.3 A π-bridge (thiophene) is inserted between the donor and acceptor unit to reduce the steric hindrance between the donor and acceptor units and to improve the planarity of the molecule. The ZOPTAN-TPA molecule features a low HOMO level of 5.2 eV and an optical energy gap of 2.1 eV. Champion OSCs based on a solution-processed and non-annealed active-material blend of [6,6]-phenyl-C61-butyric acid methyl ester (PCBM) and ZOPTAN-TPA in a mass ratio of 2:1 exhibits a power conversion efficiency of 1.9 % and a high open-circuit voltage of over 1.0 V.

Keywords : high open circuit voltage, donor, triphenylamine, organic solar cells
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