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Low Band Gap Small Molecule Acceptors for Organic Photovoltaics DAVID P. OSTROWSKI, University of Denver, UNSAL KOLDEMIR, ALAN SELLINGER, Colorado School of Mines, SEAN E. SHAHEEN, University of Colorado at Boulder and RASEI — Organic photovoltiacs (OPVs) have demonstrated solar power conversion efficiencies in the regime of 10-12% from several classes of materials, including conjugated polymers and small-molecules. Of note, in each of the classes, the electron-accepting molecule is based on C_{60}. While C_{60} is a very effective electron-acceptor and transporter, it has several non-optimal properties, including low optical absorption strength in the visible spectrum as well as the difficulty required to tune its optoelectronic properties through changes in chemical composition or substituents. Here we present results on a family of small molecule acceptors based on a core unit of benzothiodiazole (BT). The optoelectronic properties, specifically optical band gap and Lowest Occupied Molecular Orbital (LUMO), of these small molecules are readily tunable through addition of substituent groups onto the BT core. A library of these small molecule acceptors has been synthesized with broad absorbance bands of roughly 200 nm, which vary in peak absorbance from 400 nm to 640 nm. Additionally, the higher energy LUMO level of these materials, 0.3 eV higher than the C_{60} derivatives, results in OPVs with open-circuit voltages (V_{oc}) close to 1 V. The studies presented investigate overall device performance and compare the efficiencies of the two mechanisms for charge generation: channel 1 (light absorbed in donor with sequential electron transfer to acceptor molecule) and channel 2 (light absorbed in the acceptor with sequential hole transfer to donor molecule).

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