

Abstract Submitted  
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**Charge Photogeneration (CPG) in Low-Band-Gap (LBG) Donor-Acceptor (D-A) Copolymers: Higher Efficiency in LBG Polymer-Fullerene Solar Cells<sup>1</sup>** KARAN ARYANPOUR<sup>2</sup>, SUMIT MAZUMDAR<sup>3</sup>, Univ of Arizona — LBG copolymers (bandgap  $\sim 1.5$  eV) of alternating D-A moieties have attracted substantial interest in photovoltaics. Power conversion efficiency over 10% has been reported for tandem LBG copolymer-fullerene solar cells [1]. Understanding CPG in pristine LBG copolymers is a key step towards higher efficiency in LBG copolymer-fullerene solar cells. We present correlated-electron calculations within the Pariser-Parr-Pople model for excited states in LBG copolymers thieno[3,4-b]thiophene/benzodithiophene (PTB7) and poly[2,7-(5,5-bis-(3,7-dimethyloctyl)-5H-dithieno[3,2-b:2',3'-d]pyran)-alt-4,7-(5,6-difluoro-2,1,3-benzothia diazole)] (PDTP-DFBT). The goals are to understand ground state absorption, electroabsorption, and most importantly photoinduced absorptions in experiments. Of interest is the possible role of triplet excitons within the LBG donor domains in the CPG of LBG copolymers. Experiments present evidence on the high energy excited states as possible triplet-triplet (TT) combinations. While TT states in “ordinary” commonplace polymers may not play significant roles in photoinduced charge-transfer, they can possibly provide additional paths to CPG in the LBG copolymers other than the optical exciton and states close to it. [1] J. You et. al., Nat. Comm. 4, 1446 (2013)

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