Abstract Submitted
for the MAR13 Meeting of
The American Physical Society

Charge transfer excitations in water-soluble sulfonated zinc-phthalocyanine (ZnPcS) donor molecules coupled to C_{60} RAJENDRA ZOPE, LUIS BASURTO, MARCO OLGUIN, TUNNA BARUAH, University of Texas at El Paso — We present a study of charge transfer (CT) excited states for a recently synthesized group of water-soluble sulfonated zinc-phthalocyanine (ZnPcS) donor molecules coupled to C_{60}. The ZnPcS donors (ZnPcS2, ZnPcS3, and ZnPcS4) are promising materials for achieving solar cell device production with the photoactive area prepared from aqueous solution. Experimentally, decreasing the number of sulfonate substituent groups for ZnPc increased the photocurrent and lowered the open circuit voltage V_{OC}. Measurements show that the V_{OC} is largest for ZnPc-S4/C_{60} and lowest for ZnPc-S3/C_{60}. The degree of sulfonation and the measured device V_{OC} does not result in the expected pattern of values based on donor-acceptor HOMO/LUMO energy differences. Variations in film morphology may account for the unexpected pattern of V_{OC} values. Our charge transfer excited state calculations show that the lowest CT excitation energy among the group of ZnPcS/C60 donor-acceptor pairs corresponds to the disulfonated ZnPc/C60 system. The largest CT excited state energies belong to the tetrasulfonated ZnPc/C60 complex. We also examine the effect of geometrical orientation on the CT energies for the ZnPcS donor-acceptor pairs.

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Date submitted: 20 Nov 2012

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