

Abstract Submitted  
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**Synthesis and characterization of a new TPA-Thiophene based molecule for potential Organic PV applications** PRASHANT SARSWAT, University of Utah, Salt Lake City, Utah 84112, AMARCHAND SATHYAPALAN, MICHAEL FREE, University of Utah, Salt Lake City, Utah 84112 — Triphenylamine (TPA) containing molecules possess unique optical and photovoltaic properties. These molecules show very strong visible absorption due to unique electronic structure. Another class of molecules, thiophene derivatives and resulting polymers have higher hole mobility amongst other conjugate co-polymers. In view of these aspects, we have designed a new conjugated thiophene containing molecule with TPA. A solution processable technique is reported to synthesize this newly designed star shaped molecule with TPA derivative as its core and thiophene derivative as branches. The synthesized molecule is systematically characterized by studying Mass spectroscopy, Raman spectroscopy, UV-Vis spectroscopy, and cyclic voltammetry. This molecule shows solubility in various common organic solvents, broad absorption in spectral range of 300- 650 nm, and good thermal stability. An atomistic simulations based on density functional theory was carried out to validate HOMO and LUMO levels. The cyclic voltammetry analysis is consistent with atomistic simulation results. A 3D simulated orbital image reveals that the HOMO level corresponds to oxygen as well as carbon in a benzene ring.

Prashant Sarswat  
University of Utah, Salt Lake City, Utah 84112

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