ENDOHEDRAL METALLOFULLERENES AS IMPROVED ACCEPTOR MATERIALS FOR ORGANIC SOLAR CELLS

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Cost factors in inorganic solar cells have opened up a new path to less expensive manufacturing techniques using bulk heterojunction polymer/fullerene based solar cells. Using empty cage fullerene derivatives as the acceptor material, state-of-the-art organic photovoltaics currently display ~5% overall conversion efficiency. One of the main factors limiting the efficiency in organic solar cells is the low open circuit voltage. The open circuit voltage is governed by the molecular orbitals of the donor and acceptor material; therefore better matching of the orbitals will lead to improved voltages. Here we present a novel acceptor material based on Trimetasphere[®] carbon nanomaterials (TMS). Trimetaspheres[®] are endohedral metallofullerenes that consist of a trimetal nitride cluster enclosed in a C₈₀ cage. First-generation Trimetasphere[®] carbon nanomaterial derivatives have been synthesized and show behavior consistent with C_{60} but with improved molecular orbitals. Electrochemical data suggests a maximum voltage increase of up to 280 mV over C_{60} -PCBM-based devices and photophysical characterization of shows efficient and stable charge separation. Initial bulkheterojunction devices have been synthesized with open circuit voltages that are 280 mV higher than reference devices using C60-PCBM and state-of-the art (>3.4%) conversion efficiencies.