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First Principles Properties of Polymeric Photovoltaic Materials T. JAYASEKERA, J. W. MINTMIRE, Department of Physics, Oklahoma State University — Recent reports suggest that the acceptor-donor junction for bulk heterojunction photovoltaic devices can be achieved using single wall carbon nanotubes (SWNT) and polymers such as poly-3-octothiophenes (P3OT). Optical excitation is believed to occur in the organic polymer which acts as a good hole conductor, with electron transfer to the SWNT which acts as a good electron conductor. An appropriate theoretical understanding of the photovoltaic effect requires knowledge of the electronic states near the Fermi level in these materials. We calculate the electronic structure of infinitely long quasi one-dimensional nanostructures such as carbon nanotubes or electroactive chain polymers, such as polythiophenes using a first principles, all electron, self consistent local density functional (LDF) approach. We present and compare electronic structure calculations for SWNTs and poly-3alkyl-thiophenes. Further we discuss the variation of effective mass of charge carriers in polymers and SWNTs in the vicinity of Fermi level. This work was supported by the US Office of Naval Research and the DoD HPCMO CHSSI program through the Naval Research Laboratory.

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