Supporting Information for "Structural dependence of Electronic

Properties in A-A-D-A-A-Type Organic Solar Cell Material"

Ram S. Bhatta* and Mesfin Tsige*

Department of Polymer Science, The University of Akron, Ohio 44325, United States

*Corresponding authors: <u>rsb20@zips.uakron.edu</u>; <u>mtsige@uakron.edu</u>

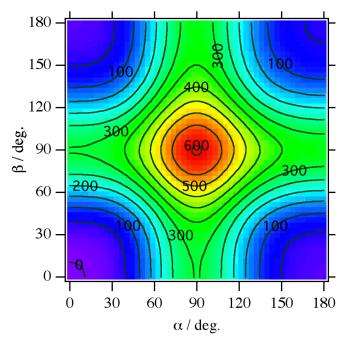


Figure S1: Contour plot of potential energy of BCNDTS molecule as a function of the two angles, α and β .

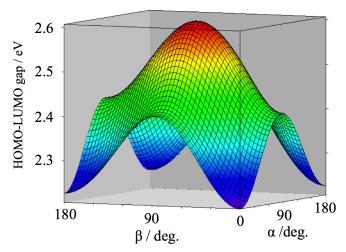


Figure S2: Two-dimensional HOMO-LUMO gap surface of BCNDTS molecule as a function of α and β .