

Abstract Submitted  
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***Ab Initio* Investigation of Conformal and Dipolar Effects on Subphthalocyanine Photovoltaic Properties** MICHAEL WATERS, GUANGSHA SHI, HOSSEIN HASHEMI, EMMANOUIL KIOUPAKIS, JOHN KIEFFER, Univ of Michigan - Ann Arbor — Boron subphthalocyanine chloride (B-SubPc-Cl) currently has the highest reported open circuit voltages of any organic photovoltaic donor coupled with C<sub>60</sub>. In our density functional theory (DFT) investigations, we sought to understand the origins of this performance by substituting boron and chlorine with other trivalent and halogen elements, respectively. Substitution of the trivalent and halogen elements distorts the porphyrin ring and changes the molecular dipole moment. For the equilibrium conformation of each isolated molecule, time-dependent DFT was used to compute the optical absorption. Using DFT with added Van der Waals interactions, experimentally unknown crystal structures were predicted. The electronic and optical excitation energies of these crystal structures were calculated using the GW/Bethe-Salpeter equation method. We found that the optical absorption spectra are significantly affected by the strong exciton binding energies in these materials ( $\sim 0.5$  eV for B-SubPc-Cl).

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