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First principles study of the electrical and optical properties of SubPc single crystal[1] XIAO MA, HOSSEIN HASHEMI, JOHN KIEFFER, Materials Science and Engineering, University of Michigan, Ann Arbor, Michigan, 48109 — We studied the electrical and optical properties of the single crystal of boron subphthalocyanine chloride (SubPc), a popular donor material used in organic photovoltaic (OPV) devices within the framework of density-functional theory (DFT) with added van der Waals long range interactions to deepen our understanding of its performance in light absorption and charge transport. We calculated the frequency-dependent dielectric response, refractive index, extinction coefficient, and intrinsic charge mobility. The complex dielectric constant was computed using first-order perturbation theory, using the electronic wave functions and eigenvalues obtained from supercell DFT calculations. This was done for wave propagation in the (001), (010), (100) directions of optimized SubPc crystal with DFT calculations, revealing significant anisotropy in both electrical and optical properties. Comparison with experimental results allows us to draw conclusions regarding the structural organization of SubPc molecules deposited on a variety of substrates, as well as the conditions for thin film growth and property optimization.

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