Abstract

Organic photovoltaic cells (OPVCs) offer a flexible and low cost alternative to traditional inorganic cells for utilizing solar energy. However, the efficiency of these devices has been considerably lower than their inorganic counterparts limiting their practicality. Therefore, building an understanding of the mechanisms at work as well as characterizing materials used in OPVCs is an important focus in utilizing solar energy. OPVCs are distinctive from their inorganic counterparts in that photoexcitiations cause the creation of excitons rather than free charge carriers. The heterojunction created by the use of specific donor and acceptor materials must be appropriate to effectively transfer the exciton to the junction and separate the electron-hole pair. One such OPVC is metal-phthalocyanine:fullerene (M-Pc:C_{60}) where M-Pc acts as the donor and fullerene the acceptor. While M-Pc crystals are generally well understood, the goal of this research is to understand spin exchange in dilute M-Pc systems where a predetermined ratio of metal to non-metal molecules is used. Density functional theory is utilized to understand the spin exchange mechanisms at work in these novel M-Pc systems to better characterize this donor material.