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Spin-orbit coupling, spin relaxation, and spin diffusion in organic solids: applications to Alq_3 and CuPc[1] ZHI-GANG YU, SRI International — We develop a systematic approach of quantifying spin-orbit coupling (SOC) and a rigorous theory of carrier spin relaxation caused by the SOC in disordered organic solids. The SOC mixes up- and down-spin in the polaron states and can be characterized by an admixture parameter γ^2. The spin mixing effects spin flips as polaron hops from one molecule to another even through the interaction that facilitate hopping is spin-indepdent. The spin relaxation time is $\tau_{sf} = \bar{R}^2/(16\gamma^2 D)$ and the spin diffusion length is $L_s = \bar{R}/4|\gamma|$, where $\bar{R}$ is the mean polaron hopping distance and D the carrier diffusion constant. We show that the SOCs in tris-(8-hydroxyquinoline) aluminum (Alq_3) and in copper phthalocyanine (CuPc) are particularly strong, due to the orthogonal arrangement of the three ligands in the former and Cu $3d$ orbitals in the latter. The theory quantitatively explains the recent observed spin diffusion lengths in Alq_3 from muon measurements and in CuPc from two-photon photoemission.

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