

MAR13-2012-000896

Abstract for an Invited Paper
for the MAR13 Meeting of
the American Physical Society

Spin-orbit coupling in organic spintronics¹

ZHI-GANG YU, SRI International

I will talk about spin-orbit coupling (SOC) in π -conjugated organic materials and its effects on spin characteristics including the spin-relaxation time, spin-diffusion length, and g factor [1]. While π electrons are responsible for low-energy electrical and optical processes in π -conjugated organic solids, σ electrons must be explicitly included to properly describe the SOC. The SOC mixes up- and down-spin states and, in the context of spintronics, can be quantified by an admixture parameter in the electron and hole polaron states in π -conjugated organics. Molecular geometry fluctuations such as ring torsion, which are common in soft organic materials and may depend on sample preparation, are found to have a strong effect on the spin mixing. The SOC-induced spin mixing leads to spin flips as polarons hop from one molecule to another, giving rise to spin relaxation and diffusion. The spin-relaxation rate is found to be proportional to the carrier hopping rate. The spin-diffusion length depends on the spin mixing and hopping distance but is insensitive to the carrier mobility. The SOC influences the g factor of the polaron state and makes it deviate from the free-electron value. The SOC strengths in common organics are quantified based on first-principles calculations and their values in tris-(8-hydroxyquinoline) aluminum (Alq₃) 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 measured spin-diffusion lengths in Alq₃ from muon spin rotation and in CuPc from spin-polarized two-photon photoemission.

[1] Z. G. Yu, Phys. Rev. Lett. **106**, 106602 (2011); Phys. Rev. B **85**, 115201 (2012).

¹This work was supported by ARO, DOE, and SRI internal funds.