

Abstract Submitted
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Spin-Orbit Induced Spin Relaxation in Organic Semiconductors¹

STEPHEN MCMILLAN, NICHOLAS HARMON, MICHAEL FLATTÉ, Univ of Iowa — Weak spin-orbit coupling suggest long spin relaxation times in organic semiconductors. The correlations between slow carrier transport and these mechanisms of spin relaxation can yield complex behavior, including large magnetic-field effects on spin and charge dynamics. We use a continuous time random walk approach to investigate the effect of spin-orbit coupling on spin relaxation in organic materials with non-interacting carriers that incoherently hop from place to place. The simulation has been adapted from earlier work in this area [1] to emphasize the quantum nature of the relaxation. Transition rates for spin conserving and spin flipping hops are calculated as functions of the randomly assigned spatial orientation of the molecular sites. In a 3D cubic lattice with nearest-neighbor hopping we observe deviations of 10% when compared to published analytic results [2]. The disparity is due to a correlation between spin flipping hops and spin conserving hops. The time that carriers spend at a given site is determined by the sum of the conserving and flipping rates. Correlations between the two types of rates affect the time between two transport events altering the relaxation time.1. N. J. Harmon and M. E. Flatté, PRB 90, 115203 (2014).2. Z.G. Yu, PRB 85, 115201 (2012).

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