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Theoretical proposal for a magnetic resonance study of charge transport in organic semiconductors[1] VAGHARSH MKHITARYAN, Ames Laboratory, Iowa State University, Ames, Iowa 50011, USA — Charge transport in disordered organic semiconductors occurs via carrier incoherent hops in a band of localized states. In the framework of continuous-time random walk the carrier on-site waiting time distribution (WTD) is one of the basic characteristics of diffusion. Besides, WTD is fundamentally related to the density of states (DOS) of localized states, which is a key feature of a material determining the optoelectric properties. However, reliable first-principle calculations of DOS in organic materials are not yet available and experimental characterization of DOS and WTD is desirable. We theoretically study the spin dynamics of hopping carriers and propose measurement schemes directly probing WTD, based on the zero-field spin relaxation and the primary (Hahn) spin echo. The proposed schemes are possible because, as we demonstrate, the long-time behavior of the zero-field relaxation and the primary echo is determined by WTD, both for the hyperfine coupling dominated and the spin-orbit coupling dominated spin dynamics. We also examine the dispersive charge transport, which is a non-Markovian sub-diffusive process characterized by non-stationarity. We show that the proposed schemes unambiguously capture the effects of non-stationarity, e.g., the aging behavior of random walks.

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