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Multi-scale modeling of spin transport in organic semiconductors SHAYAN HEMMATIYAN, Department of Physics, Texas AM University, College Station, Texas 77843, USA/Institut fur Physik, Johannes Gutenberg Universitat Mainz, Germany, AMAURY SOUZA, Institut fr Physik, Johannes Gutenberg Universitt Mainz, D-55099 Mainz, Germany, PASCAL KORDT, Max Planck Institute for Polymer Research, Ackermannweg 10, 55128 Mainz, Germany, ERIK MCNEL-LIS, Institut fr Physik, Johannes Gutenberg Universitt Mainz, D-55099 Mainz, Germany, DENIS ANDRIENKO, Max Planck Institute for Polymer Research, Ackermannweg 10, 55128 Mainz, Germany, JAIRO SINOVA, Institut fr Physik, Johannes Gutenberg Universitt Mainz, D-55099 Mainz, Germany — In this work, we present our theoretical framework to simulate simultaneously spin and charge transport in amorphous organic semiconductors. By combining several techniques e.g. molecular dynamics, density functional theory and kinetic Monte Carlo, we are be able to study spin transport in the presence of anisotropy, thermal effects, magnetic and electric field effects in a realistic morphologies of amorphous organic systems. We apply our multi-scale approach to investigate the spin transport in amorphous Alq3 (Tris(8-hydroxyquinolinato)aluminum) and address the underlying spin relaxation mechanism in this system as a function of temperature, bias voltage, magnetic field and sample thickness.

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