Abstract Submitted
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Spin-orbit couplings and spin relaxation in organic electronic materials[1] ZHI-GANG YU, SRI International — Understanding spin relaxation in organic materials requires a reliable estimate of the spin-orbit coupling (SOC) strengths in these system. It is often argued that the SOC in π-conjugated organic materials is weak because of the small atomic SOC strength of C atom. However, most organic materials used in spin transport structures, such as T_6, MEH-PPV, Alq_3, and P3HT, contain N, O, and S atoms that have a much stronger atomic SOC than C atom. Here we carry out first-principles calculation to determine the SOC strengths of several representative organic molecules. We find that in MEH-PPV and Alq3 the SOC originates mainly from the O atoms, whose lone pairs of electrons strongly couple with the C p_z orbitals. In T_6 and P3HT, the π-orbitals have a significant contribution from S atoms and therefore a sizable SOC. Using the obtained SOC strengths, we calculate the spin relaxation times and spin diffusion lengths caused by carrier hopping in these organic materials. Our results are consistent with recently measured spin relaxation times in MEH-PPV and temperature-dependent spin diffusion lengths in Alq_3.

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Zhi-Gang Yu
SRI International

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