

73. Title: Persistence time of charge carriers in defect states of molecular semiconductors

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Abstract: Charge carriers in organic crystals are often trapped in point defects. The persistence time of the charge in these defect states is evaluated by computing the escape rate from this state using non-adiabatic rate theory. Two cases are considered (i) the hopping between separate identical defect states and (ii) the hopping between a defect state and the bulk (delocalized) states. We show that only the second process is likely to happen with realistic defect concentrations and highlight that the inclusion of an effective quantum mode of vibration is essential for accurate computation of the rate. The computed persistence time as a function of the trap energy indicates that trap states shallower than similar to 0.3 eV cannot be effectively investigated with some slow spectroscopic techniques such as THz spectroscopy or EPR commonly used to study the nature of excess charge in semiconductors.