Spin Dynamics Study of Photo-Carrier Generation in TIPS-Pentacene Film by Electrically Detected Magnetic Resonance

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The spin dynamics of the electron-hole pair (e–h pair) in the photo-carrier generation is important for understanding the carrier dynamics and the performance of organic semiconductors. The aim of this study is to clarify the spin dynamics and the photo-charrier generation mechanism of the vacuum vapor deposition film of 6,13-bis(triisopropylsilyl-ethynyl)pentacene (TIPS-Pentacene) by photocurrent and electrically detected magnetic resonance (EDMR) measurement.

The TIPS-pentacene film was fabricated on a custom-made interdigitated platinum electrode by a vacuum deposition method. The photocurrent of the film sample was measured under the 1.5 V applied vias voltage and white light irradiation (100 mW) using xenon lamp. Figure 1 shows temperature dependence of EDMR spectra and the signal intensity. The intensity increased from 80 to 200 K and then decreased from 200 to 310 K. To understand the temperature dependence of EDMR, we discussed about the excited-state dynamics and carrier generation process with a model of e–h pair as illustrated in Scheme 1. The thermally active barrier was assumed from the e–h pair to carrier, which was determined to be E/k_B = 1103 K by temperature measurement of photocurrent. The temperature dependence was calculated using quantum mechanical simulations of the excited state and carrier dynamics of the e–h pair as well as the analytical solution for the kinetic rate equation using model of Scheme 1.[1]

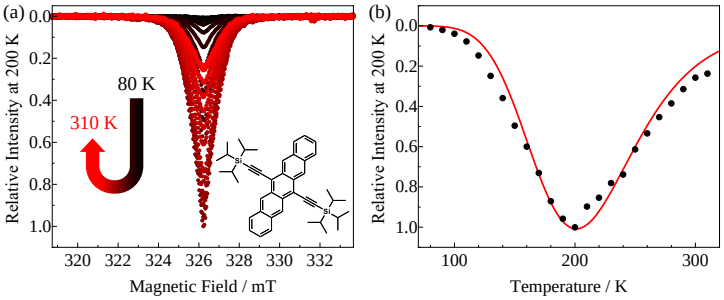
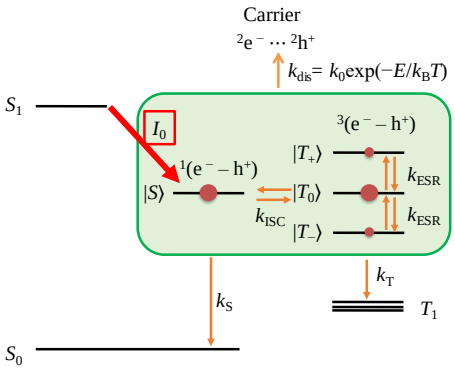


Figure 1. Temperature dependence of the photocurrent-detected EDMR. (a) EDMR spectra. (b) Temperature dependence of the signal intensity (black dots) and the simulation curve (red line).



Scheme 1. Excited-state dynamics and carrier generation process in TIPS-Pentacene film.

1) K. Kato, Y. Teki, *Phys. Chem. Chem. Phys.* **2021**, in press [DOI: 10.1039/D0CP05125J].