

W-Band ENDOR of Light-Induced PPerAcr Anion Radicals in Double-Crystalline Donor-Bridge-Acceptor P3HT- b - PPerAcr Block Copolymer in Frozen Solution: Experimental and DFT Study

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Abstract

© 2018 American Chemical Society. Light-induced W-band electron nuclear double resonance and density functional theory of a spin density distribution study of poly-perylene bisimide acrylate (PPerAcr) anion radicals in double-crystalline donor-bridge-acceptor block copolymers (BCPs) are under consideration. Evidence of spin density sharing in the electron acceptor block, mainly distributed on the perylenediimide frame of PPerAcr without delocalization along the π -stack direction of the PPerAcr block in BCPs, was found at the low (50 K) temperature in frozen o-1,2-dichlorobenzene solution. The electron-hopping frequency between the anion and the nearby neutral PPerAcr of assembled π -stacks in P3HT-b-PPerAcr BCPs is limited by a frequency of around 108 Hz at temperatures below 50 K in the steady-state regime of continuous-wave light illumination.

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