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Density of States and Trapping in Pentacene

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We show that optical and electrical measurements on pentacene single crystals can be used to extract the density of states in the HOMO-LUMO bandgap [1]. It is found that these highly purified crystals possess band tails broader than those typically observed in inorganic amorphous solids. Results on field effect transistors (FETs) fabricated from similar crystals imply that the gap state density is much larger within 5-10 nm of the gate dielectric. We also describe a defect generation phenomenon that is new to organic semiconductors [2]. A defect in pentacene single crystals can be created by bias stress and persists at room temperature for an hour in the dark but only seconds with 420nm illumination. The defect gives rise to a hole trap at $E_v + 0.38\text{eV}$ and causes metastable transport effects at room temperature. Creation and decay rates of the hole trap have a 0.67eV activation energy with a small (10^8 s^{-1}) prefactor, suggesting that atomic motion plays a key role in the generation and quenching process. [1] D. V. Lang, X. Chi, T. Siegrist, et al., Phys. Rev. Lett. 93, 086802 (2004); [2] D. V. Lang, X. Chi, T. Siegrist, et al., Phys. Rev. Lett. 93, 076601 (2004).