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**Understanding the Role of Orientational Heterogeneity on Photophysical Properties of Organic Polycrystalline Films** SAHAR SHARIFZADEH, Molecular Foundry, LBNL, CATHY WONG, HAO WU, NAOMI GINSBERG, Dept. Chemistry, UC Berkeley, LEEOR KRONIK, Dept. Materials and Interfaces, Weizmann Institute, JEFFREY NEATON, Molecular Foundry, LBNL and Dept. Physics, UC Berkeley — Organic semiconductors are a highly tunable class of optically active materials that are promising as next-generation photovoltaics. Utilizing these materials for efficient solar energy conversion relies on an understanding of the connection between their excited-state electronic structure and their solid-state morphology. While many organic materials have varying degrees of disorder, crystalline films with long-range order provide an opportunity to understand many fundamental physical properties relevant to solar energy conversion. Here, we use a combined theoretical and experimental approach to investigate the nature of low-energy excitons and their dynamics within 6,13-bis(triisopropylsilylethynyl)pentacene (TIPS-Pen) polycrystalline films. First-principles many-body perturbation theory and optical absorption spectroscopy on ordered domains reveal multiple low-energy absorption peaks that are composed of delocalized excitonic states. Further, we examine the nature of excitons in grains of different relative orientations and at grain boundaries, and discuss implications for their dynamics as measured by spatially-resolved transient absorption spectroscopy. This work was supported by DOE; computational resources provided by NERSC.

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