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Exploring the Influence of Dynamic Disorder on Excitons in Solid Pentacene[1] ZHIPING WANG, SAHAR SHARIFZADEH, Molecular Foundry, Lawrence Berkeley National Laboratory, PETER DOAK, Molecular Foundry, Lawrence Berkeley National Laboratory and Department of Chemistry, University of California, Berkeley, ZHENFEI LU, Molecular Foundry, Lawrence Berkeley National Laboratory, JEFFREY NEATON, Molecular Foundry, Lawrence Berkeley National Laboratory and Department of Physics, University of California, Berkeley — A complete understanding of the spectroscopic and charge transport properties of organic semiconductors requires knowledge of the role of thermal fluctuations and dynamic disorder. We present a first-principles theoretical study aimed at understanding the degree to which dynamic disorder at room temperature results in energy level broadening and excited-state localization within bulk crystalline pentacene. Ab initio molecular dynamics simulations are well-equilibrated for 7-9 ps and tens of thousands of structural snapshots, taken at 0.5 fs intervals, provide input for many-body perturbation theory within the GW approximation and Bethe-Salpeter equation (BSE) approach. The GW-corrected density of states, including thousands of snapshots, indicates that thermal fluctuations significantly broaden the valence and conduction states by >0.2 eV. Additionally, we investigate the nature and energy of the lowest energy singlet and triplet excitons, computed for a set of uncorrelated and energetically preferred structures.

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