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Relating Molecular-Scale Structure to Spectroscopy in Pentacene-Perfluoropentacene Donor-Acceptor Assemblies from First-Principles SAHAR SHARIFZADEH, Molecular Foundry, LBNL, LEEOR KRONIK, Weizmann Institute of Science, JEFFREY NEATON, Molecular Foundry, LBNL — Using van der Waals-corrected density functional theory and many-body perturbation theory, we compute the spectroscopic properties of the archetypal organic semiconductors pentacene (PEN), perfluoropentacene (PFP), and their composite donor-acceptor blends. Band structures, bulk crystal densities of states, and low-energy optical excitations are computed for the isolated bulk crystals and their composite assemblies. For the individual crystals, transport and optical gaps are in good agreement with experiment, and the nature and orientation of the excitonic wavefunctions is found to be sensitive to the degree of co-facial packing. For the PEN-PFP systems, different molecular arrangements and compositions are considered in an effort to connect to thin film measurements. The relationship between packing in these structures, the transport gap, and the nature and binding energies of low-lying excitons are explored. We acknowledge DOE-BES, NSF, and US-Israel BSF for support, and NERSC for computational resources.

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