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Spectroscopy of organic semiconductors from first principles SAHAR SHARIFZADEH, Molecular Foundry, LBL, ARIEL BILLER, LEEOR KRONIK, Weizmann Institute of Science, JEFFERY NEATON, Molecular Foundry, LBNL — Advances in organic optoelectronic materials rely on an accurate understanding their spectroscopy, motivating the development of predictive theoretical methods that accurately describe the excited states of organic semiconductors. In this work, we use density functional theory and many-body perturbation theory (GW/BSE) to compute the electronic and optical properties of two well-studied organic semiconductors, pentacene and PTCDA. We carefully compare our calculations of the bulk density of states with available photoemission spectra, accounting for the role of finite temperature and surface effects in experiment, and examining the influence of our main approximations – e.g. the GW starting point and the application of the generalized plasmon-pole model – on the predicted electronic structure. Moreover, our predictions for the nature of the exciton and its binding energy are discussed and compared against optical absorption data. We acknowledge DOE, NSF, and BASF for financial support and NERSC for computational resources.

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