

Abstract Submitted
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Relating Crystal Structure and the Charge-Transfer Nature of Excitons in Pentacene from First Principles¹ SAHAR SHARIFZADEH, Molecular Foundry, LBNL, PIERRE DARANCET, Molecular Foundry, LBNL and Department of Applied Physics and Applied Mathematics, Columbia University, LEEOR KRONIK, Department of Materials and Interfaces, Weizmann Institute of Science, JEFFREY NEATON, Molecular Foundry, LBNL — The nature of low energy optical excitations within pentacene has been the subject of many experimental and theoretical studies, with much disagreement as to the degree of their charge-transfer character. Here, we use many-body perturbation theory to study singlet excitons within different solid phases of pentacene and demonstrate that inter-molecular interactions lead to delocalized, charge-transfer-like excitations in the bulk crystalline phase. Using the Bethe-Salpeter two-particle correlation function, we demonstrate that the interplay between intermolecular hybridization, local exchange interactions, and attractive electron/hole interactions controls the nature of the exciton. Additionally, we explore simple models to understand and predict the nature of the excitonic wavefunction, in particular whether it has charge-transfer character.

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Sahar Sharifzadeh
Molecular Foundry, LBNL

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