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Many-Body Perturbation Theory for Understanding Optical Excitations in Organic Molecules and Solids¹
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Organic semiconductors are promising as light-weight, flexible, and strongly absorbing materials for next-generation optoelectronics. The advancement of such technologies relies on understanding the fundamental excited-state properties of organic molecules and solids, motivating the development of accurate computational approaches for this purpose. Here, I will present first-principles many-body perturbation theory (MBPT) calculations aimed at understanding the spectroscopic properties of select organic molecules and crystalline semiconductors, and improving these properties for enhanced photovoltaic performance. We show that for both gas-phase molecules and condensed-phase crystals, MBPT within the GW/BSE approximation provides quantitative accuracy of transport gaps extracted from photoemission spectroscopy and conductance measurements, as well as with measured polarization-dependent optical absorption spectra. We discuss the implications of standard approximations within GW/BSE on accuracy of these results. Additionally, we demonstrate significant exciton binding energies and charge-transfer character in the crystalline systems, which can be controlled through solid-state morphology or change of conjugation length, suggesting a new strategy for the design of optoelectronic materials.

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