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Excited-state properties of organic photovoltaic materials from a many-body Lanczos-GW approach and time-dependent density functional theory XIAOFENG QIAN, Department of Materials Science and Engineering, MIT, PAOLO UMARI, Theory at Elettra Group, CNR-INFM Democritos, Basovizza (Trieste), Italy, DAVIDE CERESOLI, NICOLA MARZARI, Department of Materials Science and Engineering, MIT — Many-body GW and time-dependent DFT (TDDFT) are two approaches that in principle allow us to access electronic and optical excited-state properties, which are critical to characterize and engineer organic photovoltaic materials. Recently we have implemented a novel approach to GW that constructs an optimal polarizability basis without using conduction states and avoids plasmon-pole approximation and sum-over-states bottlenecks using a modified Lanczos algorithm. We have also developed a real-time propagation scheme to TDDFT, able to treat large systems efficiently. We apply these two approaches to study the electronic and optical excitations in the electron acceptors often used in bulk heterojunction organic photovoltaics such as fullerene and its derivative PCBM. Our Lanczos-GW approach significantly improves upon ionization potentials and electron affinities. Optical absorption spectra for both fullerenes and PCBM from real-time TDDFT calculations are also in reasonable agreement with experimental data.

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