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Charge transfer from first principles: self-consistent GW applied to donor-acceptor systems VIKTOR ATALLA, Fritz Haber Institute, Berlin, FABIO CARUSO, University of Oxford, ANGEL RUBIO, Universidad del País Vasco, San Sebastián, Spain, MATTHIAS SCHEFFLER, Fritz Haber Institute, Berlin, PATRICK RINKE, Aalto University, Helsinki, Finland — Charge transfer in donor-acceptor systems (DAS) is determined by the relative alignment between the frontier orbitals of the donor and the acceptor. Semi-local approximations to density functional theory (DFT) may give a qualitatively wrong level alignment in DAS, leading to unphysical fractional electron transfer in weakly bound donor-acceptor pairs. *GW* calculations based on first-order perturbation theory (G_0W_0) correct the level alignment, but leave unaffected the electron density. We demonstrate that self-consistent *GW* (sc*GW*) provides an ideal framework for the description of charge transfer in DAS. Moreover, sc*GW* seamlessly accounts for many-body correlations and van der Waals interactions. As in G_0W_0, the sc*GW* level alignment is in agreement with experimental reference data. However in sc*GW*, also the electron density is treated at the *GW* level and, therefore, it is consistent with the level alignment between donor and acceptor leading to a qualitatively correct description of charge-transfer properties.

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