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Going beyond the Tamm-Dancoff approximation in the Bethe-Salpeter approach to the optical properties of solids PETER PUSCHNIG, CLAUDIA AMBROSCH-DRAXL, Atomistic Modelling and Design of Materials, University of Leoben — The solution of the Bethe-Salpeter equation (BSE) has turned out to be the method of choice for the ab-initio calculation of optical properties of semiconductors and insulators which is capable of correctly accounting for excitonic effects. Commonly, however, the coupling between the resonant and anti-resonant excitations is neglected, referred to as the Tamm-Dancoff approximation (TDA). This is well justified in many cases, in particular, for the working horses of theoretical solid state physics, such as bulk Si and GaAs. Here, we report on a first-principles investigation of the optical properties of organic semiconductors which are highly anisotropic systems. We find that the TDA no longer holds in such low-dimensional systems, where the exciton binding energies are no longer small compared to the band gaps. Going beyond the TDA leads to an increase of the exciton binding energy in the order of several tenths of an eV thereby considerably improving the agreement with experiment.

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