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Excitonic effects in molecular crystals built up by small organic molecules PETER PUSCHNIG, CLAUDIA AMBROSCH-DRAXL, University Leoben, Chair of Atomistic Modelling and Design of Materials, KERSTIN HUMMER, University of Vienna, Institute of Materials Physics, STEPHAN SAGMEISTER, University of Graz, Institute of Physics — The excitonic effects of biphenyl and 2,2'-bithiophene are investigated within an ab-initio framework. For this purpose the Bethe-Salpeter equation for the two-particle Greens function is solved. Therefrom the imaginary part of the dielectric function is derived, which includes the electron-hole interaction in the absorption process. It turns out that these organic molecular crystals, which are built by small molecules, give rise to sizeable exciton binding energies, which are between 0.7 and 0.8 eV. To study the influence of the intermolecular interaction, the exciton binding energy of crystalline biphenyl is calculated as a function of pressure. The decrease of both, the band gap and the exciton binding energy, results in a slight red-shift of the lowest optically active singlet exciton.

Peter Puschnig
University Leoben, Chair of Atomistic Modelling and Design of Materials

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