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Ab-initio calculation of excitons in conventional and anorganic semiconductors CLAUDIA AMBROSCH-DRAXL, KERSTIN HUMMER, STEPHAN SAGMEISTER, University Graz, ROBERT LASKOWSKY, NIELS CHRISTENSEN, University Aarhus, EXCITING GRAZ TEAM, EXCITING AARHUS TEAM — The excitonic effects on the optical absorption properties of organic as well as inorganic semiconductors are studied from first-principles. The Coulomb interaction between the electron and the hole is accounted for by solving the two-particle Bethe-Salpeter equation. In the organic semiconductors the exciton binding energies strongly depend on the molecular size, the crystalline packing, as well as the polarization direction of the incoming light. We show that the electron-hole interaction can lead to strongly bound excitons with binding energies of the order of 1eV or to a mere redistribution of oscillator strength. In several cases, the screening is efficient enough such that free charge carriers govern the optical absorption process. In the inorganic counterparts the sensitivity of the exciton binding energy is tested against the structural parameters and the screening of the electron-hole Coulomb interaction.

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