Interlayer Excitons and Band Alignment in MoS2/hBN/WSe2 van der Waals Heterostructures - DTU Orbit (19/01/2019)

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van der Waals heterostructures (vdWH) are ideal systems for exploring light-matter interactions at the atomic scale. In particular, structures with a type-II band alignment can yield detailed insight into carrier-photon conversion processes, which are central to, for example, solar cells and light-emitting diodes. An important first step in describing such processes is to obtain the energies of the interlayer exciton states existing at the interface. Here we present a general first-principles method to compute the electronic quasi-particle (QP) band structure and excitonic binding energies of incommensurate vdWHs. The method combines our quantum electrostatic heterostructure (QEH) model for obtaining the dielectric function with the many-body GW approximation and a generalized 2D Mott-Wannier exciton model. We calculate the level alignment together with intra- and interlayer exciton binding energies of bilayer MoS2/WSe2 with and without intercalated hBN layers, finding excellent agreement with experimental photoluminescence spectra. A comparison to density functional theory calculations demonstrates the crucial role of self-energy and electron-hole interaction effects.