First-principles theory of excitons in complex TMD- and Janus van der Waals structures

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van der Waals bonded heterostructures based on transition metal dichalcogenides or other 2D materials, represent an ideal playground for studying light-matter interactions at the nano-scale, and for benchmarking first principles excited state calculations against well defined experiments. Here we combine many-body perturbation theory with classical electrostatic models to calculate electronicstructure of the trilayer MoS2-WS2-MoSe2 and all bilayer combinations that can be obtained from combining MoS2, MoSe2, WS2 and WSe2. Band alignment and interlayer excitons are obtained using different self-energy approximations (with and without vertex corrections) and PAW-potentials (norm conserving and ultrasoft). Compared to recent experimental results we find excellent agreement with deviations of around 0.1 eV on average.

In the second part of the talk, I will discuss a novel class of ferroelectric van der Waals materials composed of stacked layers of MoSSe Janus structures. We explore the evolution of the internal electric field as function of film thickness and determine the critical thicknessbelow which the internal electric field result in the spontaneous separation of photo-excited excitons. Finally, wemdiscuss potential applications of these novel structures for photodetectors and tunneling transistors.

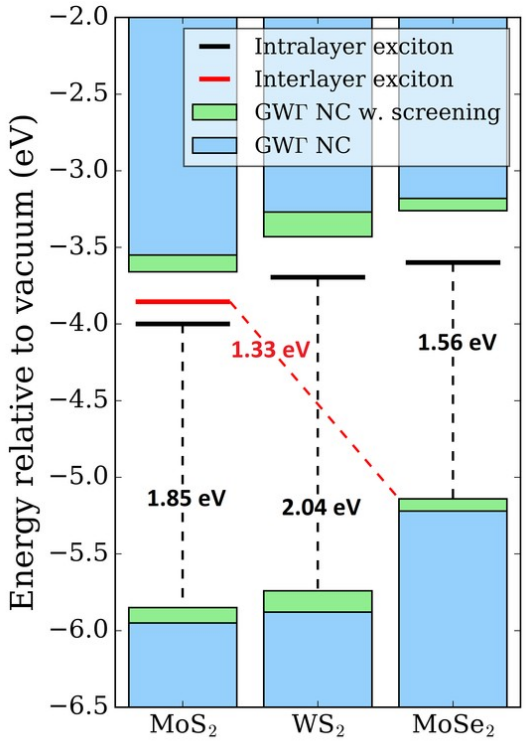

Figure 1: Band alignment and intra- and interlayer excitons of trilayer van der Waals heterostructure

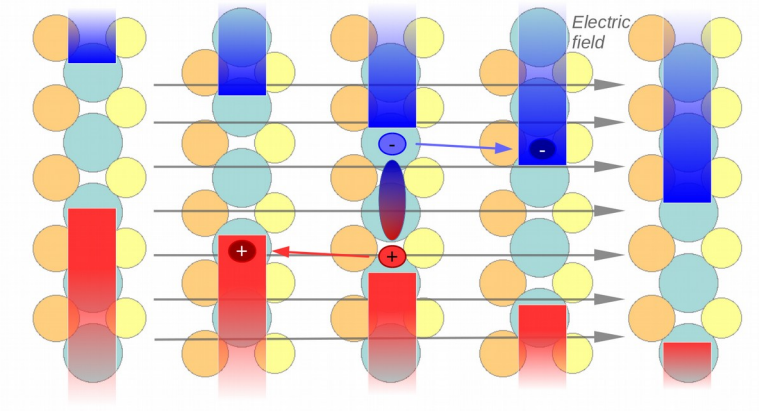

Figure 2: Band alignment and intra- and interlayer excitons of 5-layer MoSSe Janus structure