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(G) Fine Structure of Excitons in TMD Type-II Heterostructures

Monday, 6 June 2022 14:00 (15 minutes)

We describe the electronic and optical properties of MoSe2/WSe2 type-II heterostructure using *ab initio* based tight-binding (TB) approximation and Bethe-Salpeter equation (BSE) [1]. We start with determining the electronic structure of MoSe2/WSe2 from first principles. We obtain type-II band alignment and conduction band minima at Q points. Then we perform analysis of Kohn-Sham wavefunctions allowing to detect leading layer and spin contributions. Next, we construct minimal TB model for MoSe2/WSe2 heterostructure, which allow us to understand orbital contributions to Bloch states and study wavefunctions effect on excitonic spectrum. We accurately solve BSE and determine the exciton fine structure due to type-II spin-split band arrangement [2] and topological moments, considering both A/B, spin bright/dark and intra-/interlayer exciton series using simplified Rytova-Keldysh non-local screening theory. In next step we analyse effect of moiré potential and compare it with fully tight-binding approach to excitons in twisted heterostructures.

[1] M. Bieniek, L. Szulakowska, and P. Hawrylak, Band nesting and exciton spectrum in monolayer MoS2, Physical Review B 101, 125423 (2020)
[2] K. Sadecka, Inter- and Intralayer Excitonic Spectrum of MoSe2/WSe2 Heterostructure, Acta Physica Polonica, to be published (2022)

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