Finite-momentum exciton landscape in mono- and bilayer transition metal dichalcogenides - DTU Orbit (13/05/2019)

Finite-momentum exciton landscape in mono- and bilayer transition metal dichalcogenides

Monolayers and bilayers of transition metal dichalcogenides (TMDCs) are currently being intensively scrutinized not least due to their rich opto-electronic properties which are governed by strongly bound excitons. Until now the main focus has been on excitons with zero momentum. In this study we employ ab initio many-body perturbation theory within the GW/BSE approximation to describe the entire Q-resolved exciton band structure for mono- and bilayers of the MX_2 (M = Mo, W and X = Se, S) TMDCs. We find that the strong excitonic effects, i.e. strong electron-hole interactions, are present throughout the entire Q-space. While the exciton binding energies of the lowest excitons do not vary significantly with Q, we find a strong variation in their coupling strength. In particular, the latter are strongly peaked for excitons at Q = 0 and Q = Λ. For MoX_2 monolayers the K → K' excitons constitutes the exciton ground state, while in WX_2 monolayers direct transitions at K are lowest in energy. Our calculations further show that the exciton landscape is highly sensitive to strain and interlayer hybridization. For all four bilayers the exciton ground state is shifted to Γ → Λ or K → Λ transitions closely following the trends of the single-particle band structures.

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