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Electronic and optical spectra of layered semiconductors from many-body perturbation theory

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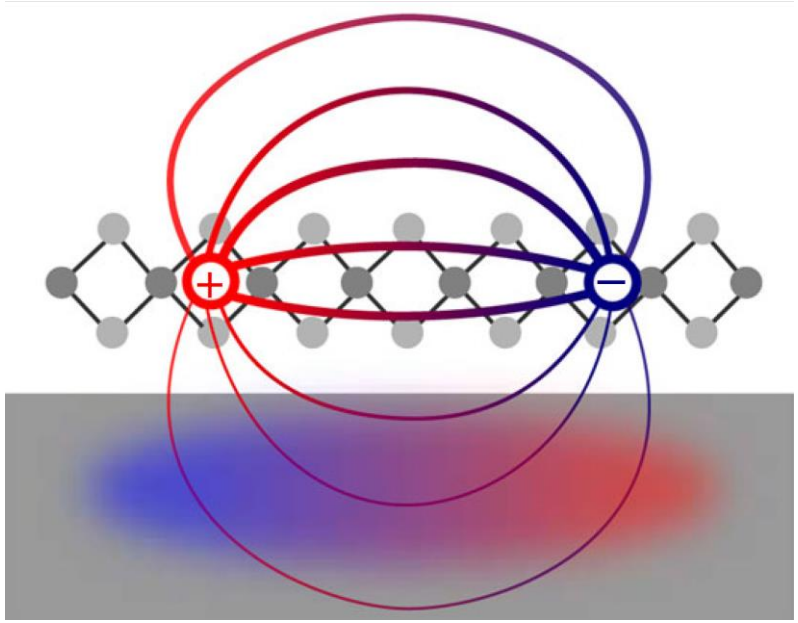

Layered semiconductors, like MoS2 or other transition-metal dichalcogenides (TMDC), exhibit particular opto-electronic properties due to their two-dimensional structure. Electronic states, like excitons, are predominantly confined to a single monolayer, but (in the case of multilayer or bulk samples) can also extend to neighbouring layers. Furthermore, they respond to charges and to dielectric polarizability in spatial vicinity, e.g. when a TMDC monolayer is deposited on a substrate.

These mechanisms can be described by ab-initio many-body perturbation theory (MBPT), notably by the GW approximation and the Bethe-Salpeter equation (GW-BSE), which can be considered as an extension of density-functional theory (DFT) to excited electronic states. The particular merit of MBPT is the incorporation of non-local dielectric screening effects on the single-particle and two-particle level.

In this talk I will give an introduction into the opto-electronic physics of TMDC materials and the role of the environment.
I will in particular discuss differences between monolayer and multilayer systems and the role of substrates.

References:
[1] M. Drüppel et al., Nature Comm. 8, 2117 (2017).
[2] Y. Niu et al., Nanomaterials 8, 725 (2018).
[3] A. Arora et al., Nature Comm. 8, 639 (2017).
[4] A. Arora et al., Nanoscale 10, 15571 (2018).