Montag, 11.04.2016 um 15.15 Uhr
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Understanding optical properties of atomically thin semiconductors from a many-body perspective

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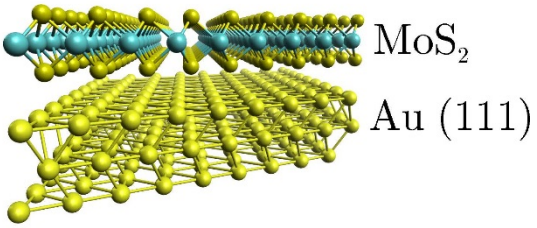
Transition metal dichalcogenides (TMDCs) open the door to a fascinating, fast growing field of two dimensional atomically thin semiconductors. This increases the demand for novel theoretical techniques, which allow to reliably calculate their optical properties. For a correct comparison with experimental results it is essential to include substrates and the correlation between more than two excited particles, i.e. trions.



We take the state of the art approach of DFT -> GW -> Bethe-Salpeter equation (BSE) and apply the efficient LDA+GdW [1] method. This enables us to describe many-body electronic excitations at moderate numerical cost.

Our results show how the optical properties of a MoS2 monolayer are modified when the screening environment is drastically changed by placing it on a substrate, or when three excited particles form a correlated trion state.

[1] M. Rohlfing, Phys. Rev. B. **82**, 205127 (2010)