Proposal for novel dark-exciton-based sensors

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Atomically thin transition metal dichalcogenides (TMDs) have been in focus of current research due to their efficient light-matter interaction and the remarkably strong Coulomb interaction leading to tightly bound excitons. Beside bright excitons, TMDs also show a variety of dark (optically inaccessible) excitons. Moreover, as TMDs are atomically thin, they are very sensitive to changes in their surrounding which opens up the possibility of externally tailoring their optical properties.

Based on a fully quantum-mechanical approach [1], we present here different strategies to control the optical fingerprint of TMD monolayers via molecules and strain. Solving the Wannier quation and the semiconductor Bloch equations on a microscopic level, we show that the coupling of excitons to high-dipole molecules can activate momentum-forbidden dark exciton states. This results in a new well pronounced resonance in optical spectra of TMDs [2] (Fig. 1). Moreover, we find that photoluminescence of these dark excitonic states is very sensitive to strain, which gives rise to significant changes in the spectral separation of dark and bright excitonic states [3]. Based on these findings, we suggest a novel mechanism for optical sensing of molecules and strain through activation of dark excitonic states in atomically thin 2D materials.

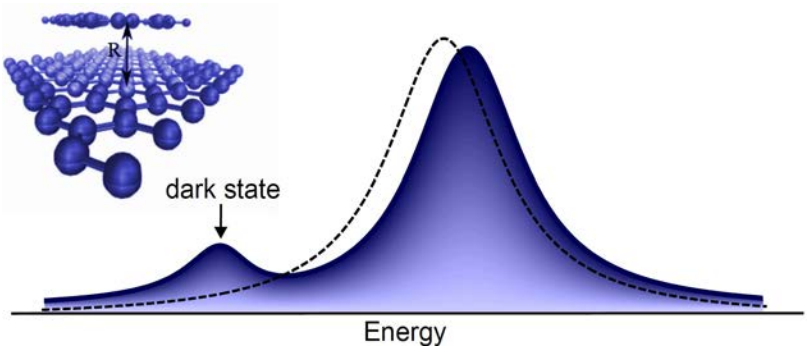

Fig.1. Excitonic absorption spectrum of pristine (dashed) and molecule-functionalized (blue filled) tungsten disulphide (WS_2). The presence of high-dipole molecules activates dark excitons resulting in a new resonance at the lower energy side of the bright exciton.

[1] M. Selig, G. Berghaeuser, A. Raja, P. Nagler, C. Schueller, T. Heinz, T. Korn, A. Chernikov, E. Malic, and A. Knorr, Nat. Comm. **7**, 13279 (2016).

[2] M. Feierabend, G. Berghäuser, A. Knorr, and E. Malic, Nat. Comm. **8**, 14776 (2017).

[3] M. Feierabend, Z. Khatibi, G. Berghäuser, and E. Malic, arXiv: 1806.07350 (2018)