

Controlling the optical fingerprint of transition metal dichalcogenides via molecules, strain and disorder

Maja Feierabend¹ and Ermin Malic¹

¹Department of Physics, Chalmers University of Technology, 41296 Gothenburg, Sweden

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.

Here, based on a fully quantum-mechanical approach, we present different strategies to control the optical fingerprint of different TMD monolayers via molecules, strain or impurities. We show that the coupling of excitons to specific molecules can activate momentum-forbidden dark exciton states resulting in an additional well pronounced peak in the optical spectra [1,2] (Fig. 1). Moreover, we find that these dark excitonic states are very sensitive to strain, leading to crucial energy shifts and intensity changes of dark exciton signatures (Fig. 1). Based on these findings, we suggest a novel optical sensing method for molecules and strain through activation of dark excitons. Finally, we also investigate which impact disorder has on the formation of localized excitonic states including their excitonic binding energies, phonon-assisted capture processes and thermalization as well as their photoluminescence including the possibility of single-photon emission [3].

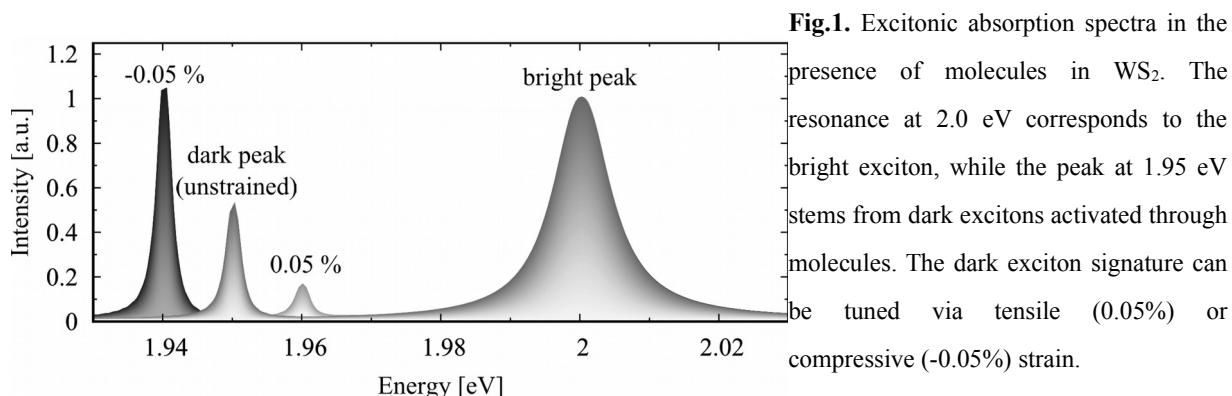


Fig.1. Excitonic absorption spectra in the presence of molecules in WS₂. The resonance at 2.0 eV corresponds to the bright exciton, while the peak at 1.95 eV stems from dark excitons activated through molecules. The dark exciton signature can be tuned via tensile (0.05%) or compressive (-0.05%) strain.

- [1] M. Feierabend, G. Berghäuser, A. Knorr, and E. Malic, Nat. Comm. **8**, 14776 (2017).
- [2] M. Feierabend *et al.* Phys. Rev. Materials **2**, 014004 (2018)
- [3] M. Koperski *et al.* Nat. Nano. **10**, 503-506 (2015)