Optical signals of qubits in defected 2D TMDs

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Abstract

The coupling between spin and valley degrees of freedom is one of the most intriguing properties of transition metal dichalcogenides (TMDs). This effect allows us to populate a single spin and valley combination using a circularly polarised laser. However, it has been shown that intrinsic properties alone cannot sustain long lived spin signals and that these must come from extrinsic properties [1]. Among the latter, defects offer the possibility to enrich the optical properties of TMDs. Vacancies and impurities are present in non-negligible concentrations even in the best high-quality samples. In this work we link different types of defects to specific optical signatures by employing many-body perturbation theory with the Yambo package [2] to obtain the optical absorption spectra of defected transition metal dichalcogenides.

We find that the largely unstudied metal vacancies show a larger set of polarized excitons than chalcogen vacancies, introducing localized excitons in the sub-optical-gap region [3] whose wave functions and spectra make them good candidates as quantum emitters. However, when dealing with substitutional defects, the spin texture and pristine exciton energies are preserved, despite the strong interaction with the defect. Nevertheless, as the full optical-gap region remains free, these defects can be used as sites for grafting and patterning in optical detectors. A redistribution of excitonic weight between the A and B excitons is visible in both cases and may allow the quantification of the defect concentration. This work establishes excitonic signatures to characterize defects in 2D materials and highlights vacancies as qubit candidates for quantum computing.

References

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[2] D. Sangalli, et al, Journal of Physics: Condensed Matter 31 (2019), 325902
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Figures

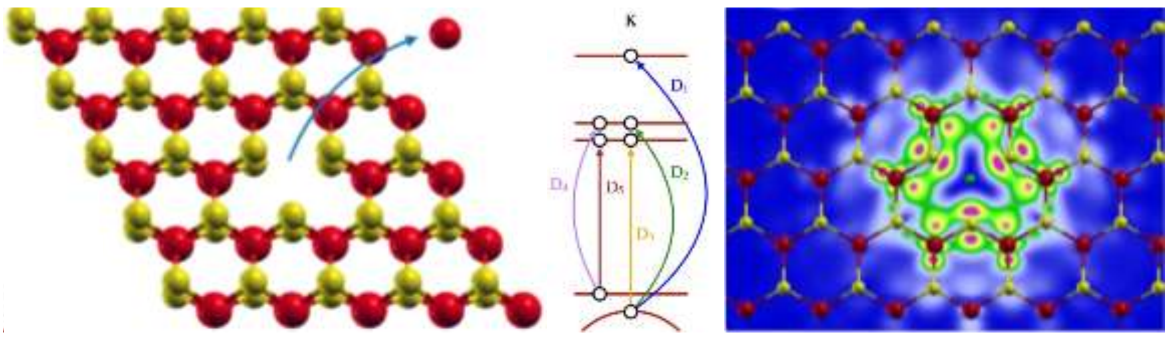

Figure 1: Removal of a tungsten atom introduces new, middle gap states in electronic band structure, even below the Fermi energy. These new defect-bound valence and conduction states form new, highly localized excitons, making them good candidates for qubit systems.