OPTICAL SIGNALS OF QUBITS IN DEFECTED 2D TMDS

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Hard to avoid even in the best quality samples of 2D materials, vacancies and impurities are often present, even at non-negligible concentrations[1,2]. Their presence will alter intrinsic properties, so it becomes crucial to understand how we can take advantage of the presence of defects to generate functionality. In this work we employ many-body perturbation theory to obtain the optical absorption spectra of defected transition metal dichalcogenides using the yambo code[3]. New optical features arise in the presence of vacancies, especially in the largely unreported metal vacancies[4]. These show a large manifold of sub-optical-gap excitons, whose wave-functions are highly localized, making them good candidates for quantum dots. For the cases where isovalent substitutional defects are present, both the spin texture and the pristine excitonic energies are preserved, despite the strong interaction with the defects. There is, however, some redistribution of spectral weight between the A and B excitons which is visible in both cases and may allow for the quantification of the defect concentration. With this work we establish how excitonic signatures characterize defects in 2D materials and highlight vacancies as qubit candidates for quantum computing.

References

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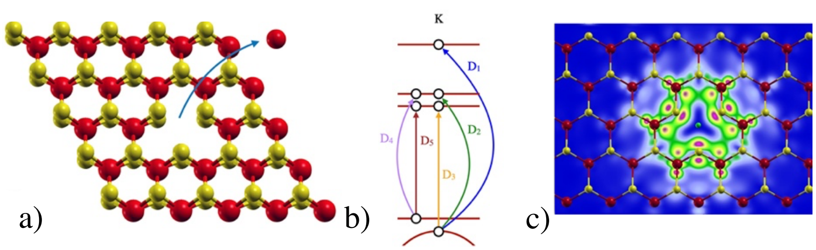

Figure 1: Removal of a tungsten ion (a) on a WS_2 monolayer leads to new, defect-bound in-gap states (b) in the electronic structure. These are responsible for new optical features in the absorption spectrum and lead to the formation of strongly localized qubits (c).

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