Quantum Materials optolelectronics

Z. Zanolli

Utrecht University, Princetonplein 1, 3584 CC Utrecht, The Netherlands

z.zanolli@uu.nl

Controlling the properties of quantum materials via external stimuli is a key topic in modern condensed-matter physics. Due to its intrinsic quantum nature, light plays several roles: generating and controlling excited states, and forming hybrid quasiparticles with other excitations in solids. To unlock quantum advantage in electronic, photonic and energy technologies it is required to create new materials and manipulate their properties. To reach this goal we develop theory and simulation techniques to fully describe the interaction between light (photons), bound electron-holes pairs (excitons) and lattice vibrations (phonons) without adjustable parameters in a quantum many-body framework [1]. Using this approach, we compute optical properties of 2D materials and heterostructures and predict how these properties can be controlled by defect engineering, strain, or twisting. For instance, we find that vacancies in Transition Metal Dichalcogenides can univocally be identified by their absorption spectra and used as carriers of quantum information [2]. Further, we demonstrate the essential role played by exciton-phonon interaction in photoluminescence of negatively-charged boron vacancy in 2D hexagonal boron nitride [3], in achieving long spin-relaxation times in TMDs [4], and in characterizing the valley profile in TMDs [5]. We find intralayer and interlayer excitons in TMD heterostructures and use twisting to tune their absorption energy. Tunable materials are promising platforms for application in quantum information, quantum sensing, and quantum transport.

References

[1] D. Sangalli, *et al.*, J. Condens. Matter Phys. **31** (2019) 325902

[2] P.M.M.C. de Melo, Z. Zanolli, M. J. Verstraete, Adv. Quantum Technol. **3** (2021) 2000118

[3] F. Libbi, P.M.M.C. de Melo, Z. Zanolli, M. J. Verstraete, N. Marzari, Phys. Rev. Lett. **128**, 167401 (2022)

[4] M. Ersfeld, *et al.* Nano Lett. **196**, 4083-4090 (2019).

[5] T. Sohier, P. M.M.C. de Melo, Z. Zanolli, M. J. Verstraete, 2D Mater. **10**, 025006 (2023)

Figures

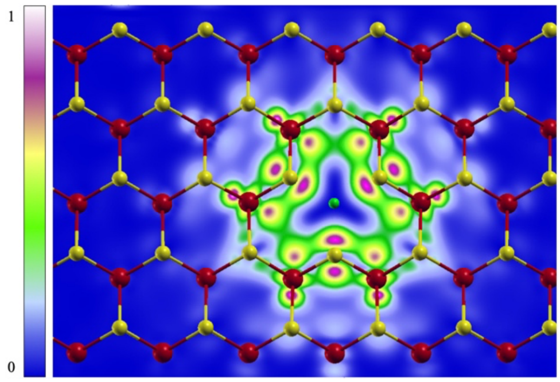

Figure 1: Excitonic wavefunction for an excitonic state localized on a W vacancy in WS_2. The electronic charge is highly localized near the missing W atom, indicating the formation of a quantum dot. Ref. [2]

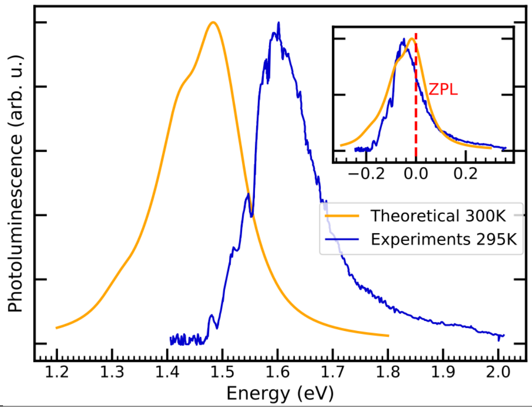

Figure 2: Theoretically predicted phonon-assisted luminescence normalized and compared to experiments. The insets shows the theoretical and experimental curves after aligning the zero phonon lines (ZPLs). Ref. [3]