Optically active self-organised quantum dots in marginally twisted $MoSe_2/WSe_2$ and MoS_2/WS_2 bilayers

Vladimir Falko
National Graphene Institute, University of Manchester, M13 9PL, Manchester, UK
vladimir.falko@manchester.ac.uk

Moiré superlattices in twistronic heterostructures are a powerful tool for materials engineering. In marginally twisted (small misalignment angle, ϑ) bilayers of nearly lattice-matched two-dimensional (2D) crystals moiré patterns take the form of domains of commensurate stacking, separated by a network of domain walls (NoDW) with strain hot spots at the NoDW nodes. Here, we show[1] that, for type-II transition metal dichalcogenide bilayers MoX_2/WX_2 (X=S, Se), the hydrostatic strain component in these hot spots creates quantum dots for electrons and holes. We investigate the electron/hole states bound by such objects, discussing their manifestations via the intralayer intraband infrared transitions. The electron/hole confinement, which is the strongest for ϑ <0.5°, leads to a red-shift of their recombination line producing single photon emitters (SPE) broadly tunable around 1.2 eV by misalignment angle. These self-organised dots can form in bilayers with both aligned and inverted MoX_2 and WX_2 unit cells, emitting photons with different polarizations. We also find that the hot spots of strain reduce the intralayer MoX_2 A-exciton energy, enabling selective population of the quantum dot states.

References

[1] V. Enaldiev, F. Ferreira, J. McHugh, V. Fal'ko, arXiv:2204.06823

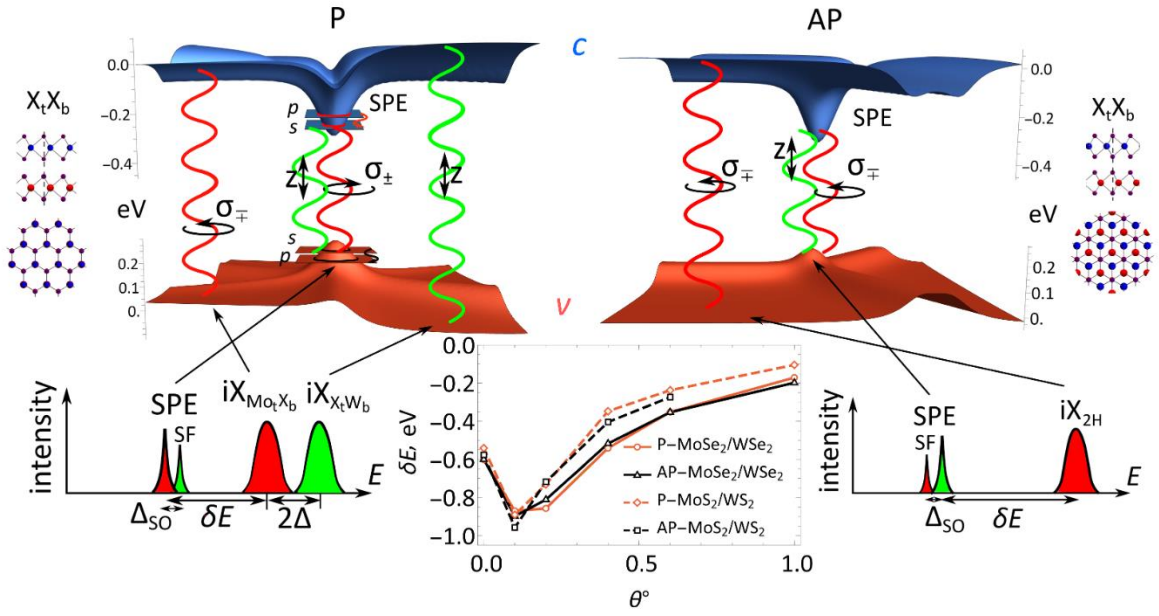

Figure 1: Self-organised quantum dots and spectral features of SPE and the interlayer excitons, iX. (Top) Conduction (c) and valence (v) band edge profiles in vicinity of X_tX_b nodes of the network of domain walls in a reconstructed P- and AP-MoX_2/WX_2 bilayers with θ = 0◦. Colors of wavy lines encode polarisations of emitted light in ±K-valleys: red for circular and green for z-polarisation. Upper/lower subscript of circular polarisation ($\sigma^{\pm}$ or $\sigma^{\mp}$) indicates helicity of light emitted in +K/−K-valleys. Left and right bottom panels show sketches of predicted optical spectra in marginally twisted P- and AP-MoX_2/WX_2 bilayers, respectively. Middle bottom panel shows the calculated shift of the SPE energy (3) with respect to energy of iX inside of Mo_tX_b/2H domains for P- and AP- bilayers.