Moiré superlattice excitons in heterostructures of transition metal dichalcogenides

Vladimir Fal'ko

National Graphene Institute
University of Manchester
M13 9PL, Manchester, UK

vladimir.falko@manchester.ac.uk

Atomically thin layers of 2D materials can be assembled in vertical stacks held together by relatively weak van der Waals forces, allowing for coupling between monolayer crystals with incommensurate lattices and arbitrary mutual rotation. A profound consequence of using these degrees of freedom is the emergence of a periodicity in the local atomic registry of the constituent crystal structures, known as a moiré superlattice. Here, we discuss how moiré superlattice effects on the electronic properties of almost aligned, e.g., $MoSe_2/WS_2$ and $MoTe_2/MoSe_2$ heterobilayers get enhanced by resonant hybridization of conduction-band states in different layers, promoted by alignment of their band edges [1]. In particular, we find that in semiconducting heterostructures built of incommensurate $MoSe_2$ and WS_2 monolayers, An exciton undergoes an almost resonant interlayer hybridisation, resulting in the enhancement of the moiré superlattice effects, [1] as an electron in the exciton explores efficiently the local arrangement of atoms in the two layer. $MoSe_2$ and WS_2 are specifically chosen for the near degeneracy of their conduction band edges to promote the hybridisation of intra- and interlayer excitons, which manifests itself in photoluminescence through a pronounced exciton energy shift as a periodic function of the interlayer rotation angle [2]. This occurs as hybridised excitons (hX) are formed by holes residing in $MoSe_2$ bound to a twist-dependent superposition of electron states in the adjacent monolayers. For heterostructures with almost aligned pairs of monolayer crystals, resonant mixing of the electron states leads to pronounced effects of the heterostructure's geometrical moiré pattern on the hX dispersion and optical spectrum, with new lines in their optical absorption spectra that correspond to the electron-photon umklapp processes [1,2]. Depending on the orientation (parallel or 2H), similar resonant hybridization is possible for B excitons in some TMD heterostructures, and that they should naturally appear in twisted homobilayers of TMDs.

[1] D. Ruiz-Tijerina & V. Fal'ko, Phys. Rev. B 99, 125424 (2019)

[2] E. Alexeev, et al, Nature 567, 81 (2019)

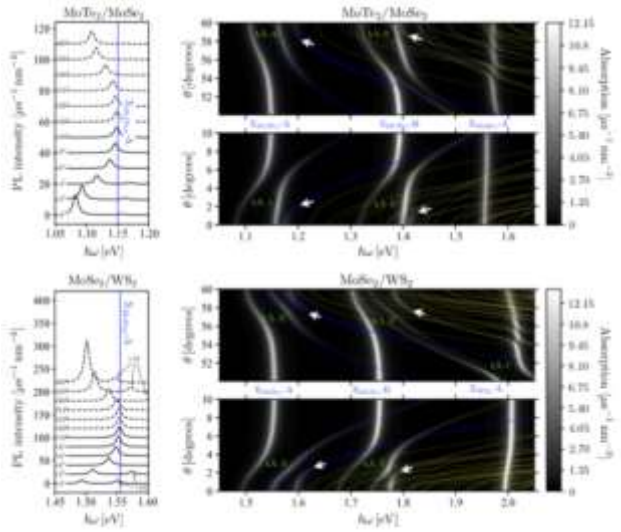

Figure 1: Absorption by mire excitons in TMD heterostructures with almost resonant band edges.