# Twisted-angle dependent exciton in heterobilayer of transition metal dichalcogenides

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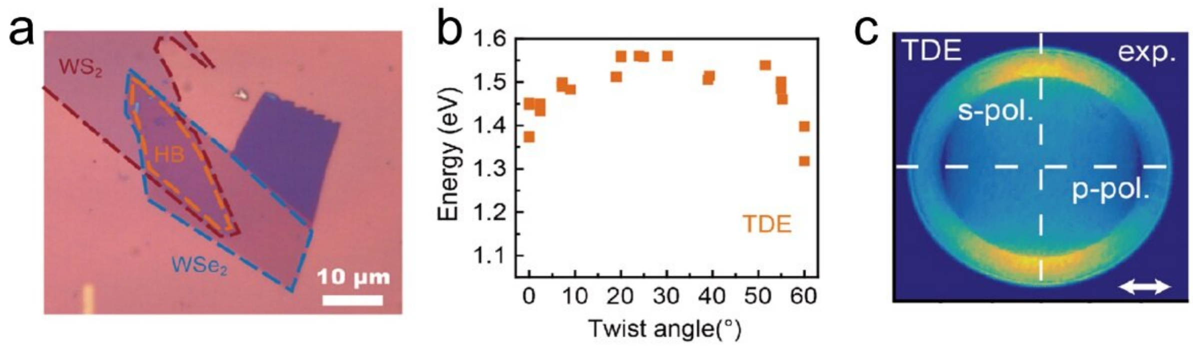


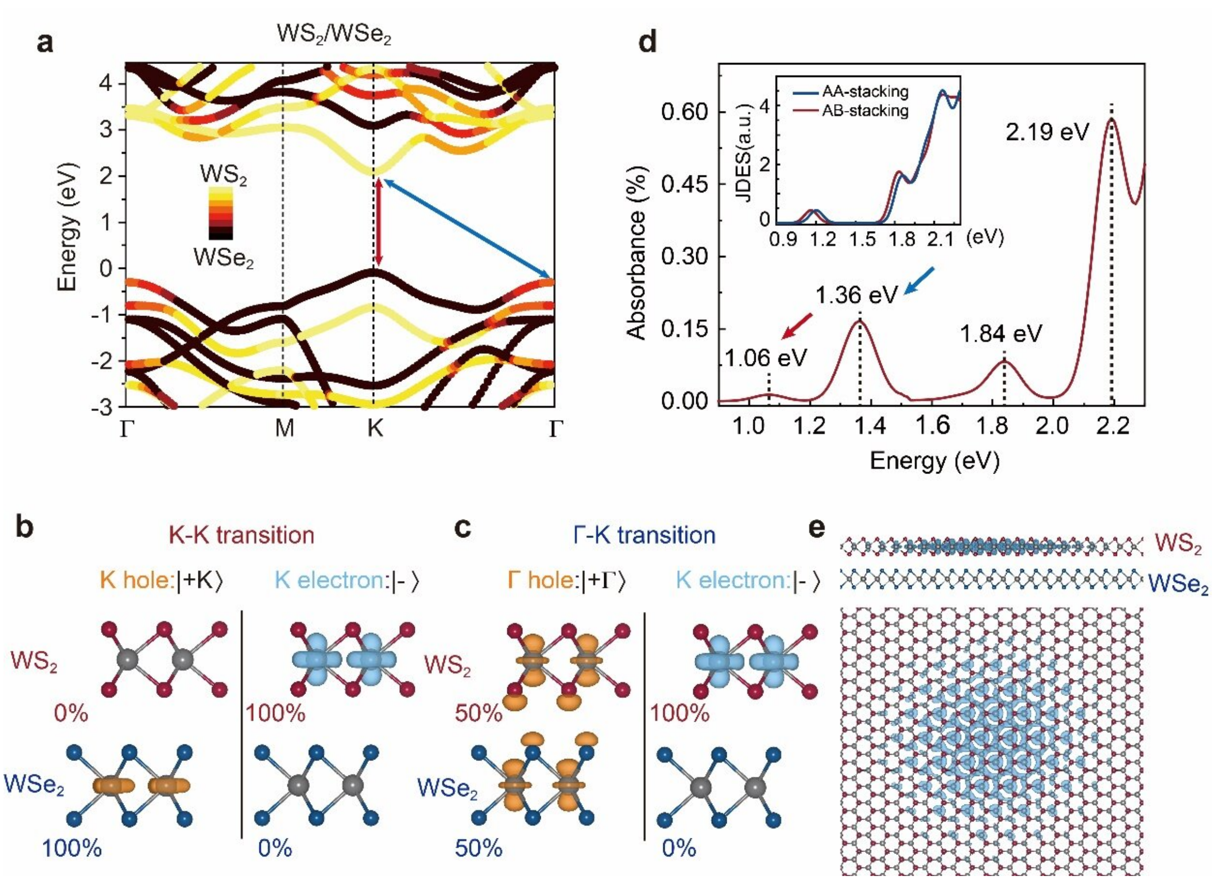

(a) Optical image of $WS_2/WSe_2$ heterobilayer. (b) The energy of the TDE in $WS_2/WSe_2$ heterobilayer as a function of twist angle. (c) The polarized k-space emission pattern of the TDE. Credit: Science China Press

The type-II band structures in vertically stacked transition metal dichalcogenides (TMDs) heterobilayers facilitate the formation of interlayer excitons. The twist-angle and the mismatch in the lattice constants of the monolayers create a periodic moiré potential as deep as >100 meV, which can affect the optical bandgap and the optical selection rules of the forming excitons. Identifying the origin of the exciton peaks in TMDs heterobilayers is sometimes controversial because their similar energies.

Recently, researchers from Wuhan University (Nanophotonics Group led by Prof. Shunping Zhang and Prof. Hongxing Xu, Computational Physics Group led by Prof. Shengjun Yuan) show that a twist-angle dependent exciton (TDE) resulted from interlayer coupling between monolayer WS2 and WSe2, is an intralayer exciton with its transition dipole moment almost parallel to the atomic plane. They identify this exciton based on a systematic analysis and comparison of experimental PL spectra, twist-angle dependent DFT band structure calculations, more accurate DFT-GW calculations, and the state-of-art optical calculations using the GW-BSE approach.

The experiments show that the new exciton at around 1.35 eV in WS2/WSe2 heterobilayers depends on the twist angle (Figure 1b), exhibiting the charactersitcs of the so-called "interlayer exciton". Then they used the back focal plane imaging (Fourier imaging) technique to quantify the orientation of the transition dipole moment of the TDE in $WS_2/WSe_2$ heterobilayer in Figure 1c. The *k*-space emission pattern of the TDE shows an in-plane dipole character, independent of the twist angle.

Further analysis indicates that this "interlayer exciton" is indeed an intralyer exction contributed from $WS_2$ layer, and the major evidence includes: (1) The comparision of the experimental PL spectra and the calculated absorption spectrum (Figure 2d) show that the 1.35 eV in the PL spectra matches well with the calculated 1.36 eV; (2) The momentum indirect transition character of 1.36 eV peak in the optical absorption spectrum have also been validated by the zero-joint density of excited states (Figure 2d) around 1.36 eV; (3) The excitonic weight analysis clearly shows that the exciton state 1.36 eV is mainly caused by the transition Γ-K; (4) The analysis of real-space distribution of the charge density of the exciton 1.36 eV (Figure 2e) shows that both the electron and hole come from the $WS_2$ layer only.




(a) The band structure of $WS_2/WSe_2$ heterobilayers. (a, b) The distribution of the hole |+⟩ and electron |–⟩ states associated with (b) the K-K excitation and (c) the Γ-K excitation. (d) The optical absorption spectra of WS2/WSe2 heterobilayers. (e) The real-space distribution of the charge density in the TDE. Credit: Science China Press

**More information:** Ke Wu et al, Identification of twist-angle-dependent excitons in $WS_2/WSe_2$ heterobilayers, *National Science Review* (2021). [DOI: 10.1093/nsr/nwab135](https://dx.doi.org/10.1093/nsr/nwab135)

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