

Control of WS₂ emission properties in 2D-3D semiconductor heterojunctions by band alignment

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During the last years transition metal dichalcogenides (TMDCs) have been established as promising building blocks of van der Waals (vdW) heterostructures. In contrast to heterostructures grown by epitaxy, vdW layers can be combined principally without restrictions given by lattice type and mismatch. This opens on the one side fascinating approaches for combining semiconducting TMDCs with other conducting, semiconducting or insulating 2D materials for applications e.g. in nm-thick LEDs, solar cells or photodetectors. On the other side, 2D materials can serve as tailored functional layers on top of classical bulk semiconductors to implement novel optoelectronic devices [1]. However, experimental research about the impact of semiconducting substrates on TMDC layer luminescence is still at a very initial state: It is not clear, to what extend the classical models describing semiconductor heterojunctions can be transferred to layers with atomic thickness with their specific band structure.

We study mechanically exfoliated WS₂ monolayer flakes on GaN substrates with different doping levels for getting fundamental insights into the charge transfer mechanism between 2D materials with a direct bandgap at the K point and 3D materials with a direct bandgap at the Γ point. By using a GaN wide-gap substrate we are able to alter the band alignment between WS₂ and the substrate drastically by doping, as the GaN Fermi level can be shifted by more than 1.5 eV between i-GaN and highly p-doped material. An appropriate choice of excitation wavelength allows carrier generation purely in the WS₂ layer.

Under green excitation ($\lambda = 532$ nm), no significant change of the WS₂ photoluminescence (PL) is found for different doping levels (Fig.1, left). The picture is fundamentally different for blue excitation ($\lambda = 405$ nm), where the PL is completely quenched in case of a highly p-doped substrate (doping level nearly $10^{19}/\text{cm}^3$). In order to explain these findings we have to be aware that by increasing the p doping level, the GaN valence band is shifted energetically above the WS₂ valence band at the Γ point, in principle enabling charge transfer from the 2D to the 3D material. In case of excitation at $\lambda = 532$ nm, carriers are generated mainly at the K point of WS₂. Obviously, charge transfer from the K point of WS₂ to the GaN substrate is widely suppressed. In contrast, under blue excitation ($\lambda = 405$ nm) a large number of carriers is created close to the Γ point in the Brillouin zone because of the band nesting (inset in Fig. 1) [2]. These holes can apparently overcome the 2D-3D heterojunction in case of p-GaN, strongly quenching the WS₂ PL signal. Consequently this carrier transfer mechanism should be blocked by adding an insulating layer between WS₂ and the substrate. We confirm this by introducing a 2D insulator (8 nm hBN) beneath the WS₂ flake, leading to a recovery of the initial WS₂ photoluminescence (Fig. 1 right).

References

[1] Tsai et al., ACS Nano **8**, 8317 (2014)

[2] Kozawa et al., Nat. Comm. **5**, 4543 (2014)

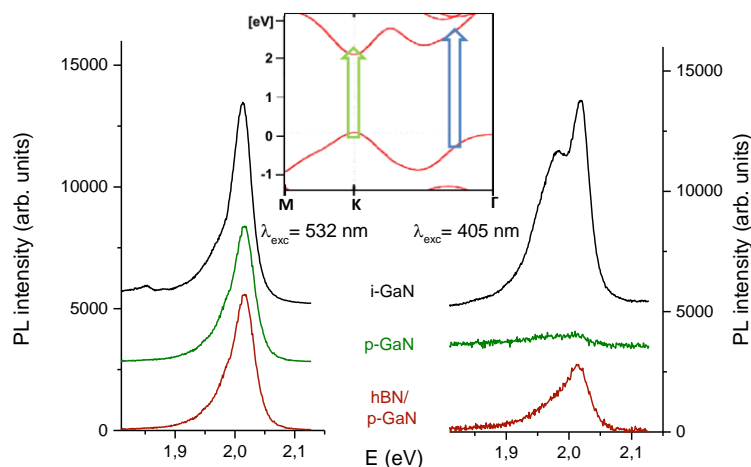


Fig. 1: Photoluminescence of WS₂ monolayers on top of differently doped GaN substrates. Excitation was performed close to the K point ($\lambda = 532$ nm, left) and close to the Γ point ($\lambda = 405$ nm, right) in the band nesting region [2]. The PL signals on p-GaN are measured on the same WS₂ flake that partly overlaps with hBN while the other part is in direct contact with the substrate.