Noble TMDs heterostructures based devices

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The possibility of combining different materials to obtain a tailor-made ultra-thin heterostructure is a peculiarity and an advantage of two-dimensional (2D) materials. Among them, the so called noble-transition-metal dichalcogenides (TMDs) stand out for their exceptionally bandgap dependence on stacking order, which can also lead to a change of fundamental electronic properties (from metal to semiconductor) [1]. Recently, some of these materials have been synthesized in mono- and few-layers and exploited in the realizations of Field Effect Transistors (FETs) [2-4]. By means of muti-scale simulations, we explore the potential of new device concepts based on PdS_2, PtS_2 and NiS_2 lateral heterostructures (LH), which operate either as Schottky Barrier (SB) or as standard FETs. We will show that PdS_2 and PtS_2 based devices show a very promising behaviour, compliant with industry requirements for low power and high-performance applications.

References

[1] P. Miro et al., *Angew. Chem.*, **53**, 3015 (2014)
[2]A. Ciarrocchi et al., *Nat. Comm.*, **9**, 919 (2018)
[3]Y. Zhao et al., Adv. Mater., **29**, (2017)

[4] C. Yim et al., *npj 2D Materials and Applications*, **2,** 5 (2018)

Figures

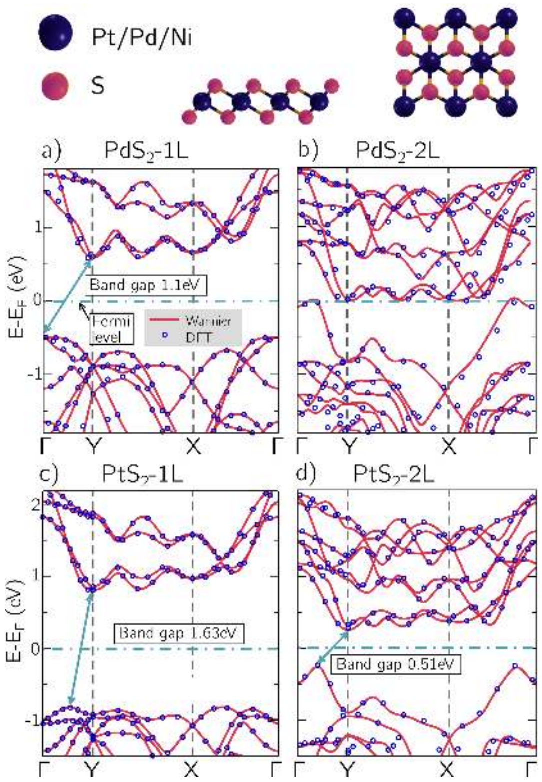

Figure 1: Electronic band-structure for mono-layer and bilayer PtS2 and PdS2 as calculated with Density functional theory (circles) and with Maximally Localized Wannier Functions (lines). On top:1T-crystal structure, lateral and top view.

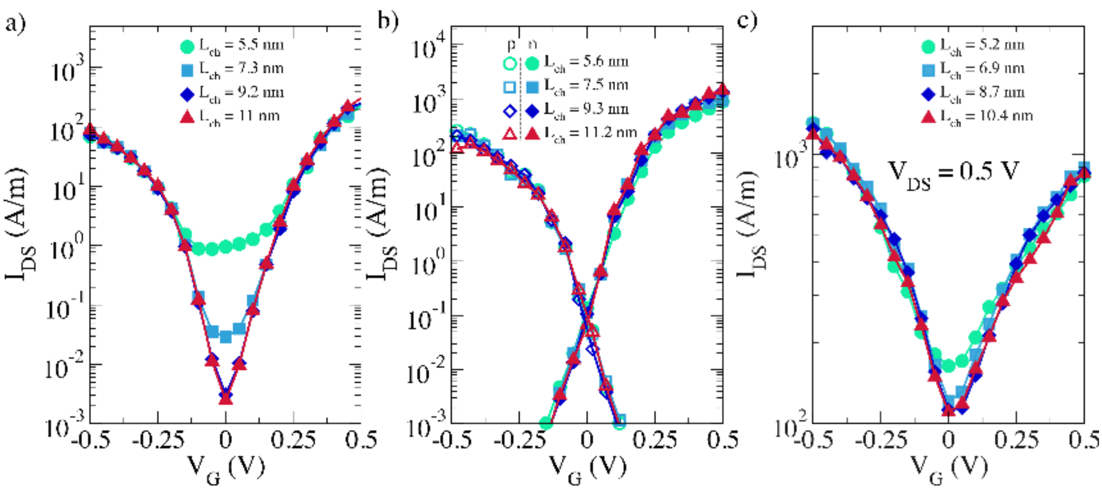

Figure 2: Transfer characteristic (semi-logarithmic scale) for LH-FETs with channel lengths ranging from 5 nm up to 10 nm made of PdS_2 (a), NiS_2 (b) and PtS_2 (c). The drain-to-source voltage V_{DS} is 0.5 V