Work Function Modulation in Semimetal-based Contact Stacks for p-type TMD FETs

Alfonso Sanchez-Soares[1], Thomas Kelly[1], James C. Greer[2] and Giorgos Fagas[3]
[1]*EOLAS Designs Ltd, Cork, Ireland.* [2]*University of Nottingham, Ningbo, China.*
[3]*Tyndall National Institute, UCC, Lee Maltings, Cork, Ireland*
alfonso.sanchez@eolasdesigns.com

Transition metal dichalcogenides (TMDs) comprise the most promising material class for post-silicon field-effect transistors at sub-10 nm gate lengths. Recent advances in process engineering and device design have been steadily bringing TMD-based technology closer to commercial applications [1]. One remaining challenge is the realization of contacts with low resistance at interfaces between TMDs and source/drain electrodes. For n-type devices, the introduction of a semi-metal layer between the metal electrodes and TMDs has proven successful in achieving contact resistances competitive with silicon-based technology [2,3]. Similar contacts for p-type devices remain elusive due to unfavourable band alignments between TMDs and suitable semimetals. A recent study proposed exploiting confinement effects thin semimetal films to modulate the work function of contact stacks and thus reduce p-type contact resistance to WSe_2 [4]. This work applies a quantum transport simulation methodology previously calibrated to reproduce the characteristics of n-type semimetal contacts to MoS_2 to build on that concept [5]. We study contact stacks comprised of metals with varying work functions and a semimetal layer with thickness below 5 nm. We simulate the electrical characteristics of devices arranged in back-gated architectures typically employed in experimental characterization of similar contact stacks. Results elucidate the most relevant physical mechanisms at play at contact interfaces and provide insight into considerations for semimetal-based contact design.

References

[1] O'Brien K.P., Naylor C.H., Dorow C. *et al.*, Nature Communications 14 (2023) 6400
[2] Shen PC., Su C., Lin Y. *et al.*, Nature, 593 (2021) 211-217
[3] O'Brien K.P. *et al.*, IEEE International Electron Devices Meeting (2021) 7.1.1-7.1.4
[4] Nakajima R. *et al.*, ACS Applied Electronic Materials, 6 (2024) 144-149
[5] Sanchez-Soares A. *et al.*, Solid State Electronics, *Under Review* (2025)

Figures

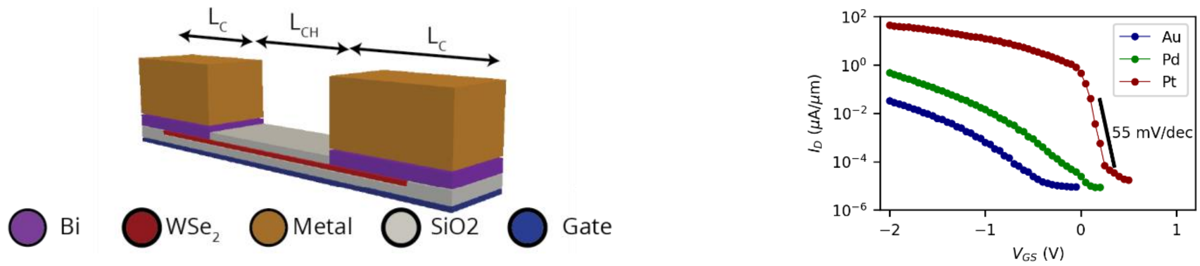

Figure 1: Device geometry with contact stacks comprised of a metal and Bi (left), and transfer characteristics for varying metals in the contact stack (right).

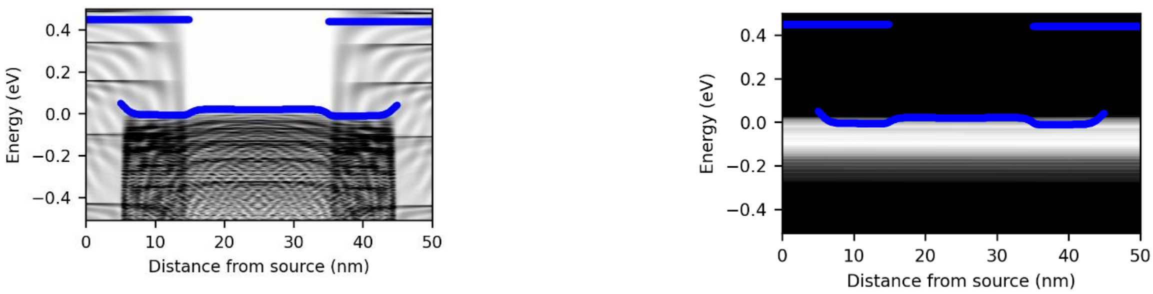

Figure 2: Local density of states (left) and spectral current (right) for a device with Pt/Bi contacts.