Work-Function Engineering in Ultra-Scaled 2D-TFET Devices: An Atomistic DFT-NEGF Study

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Two-dimensional (2D) materials such as transition metal dichalcogenides (TMDs) have recently been included in the International Roadmap for Devices and Systems (IDRS) as promising channel materials for next-generation sub-10nm technology nodes [1,2]. In this contribution, we investigate the electrical characteristics of an ultra-scaled tunnel FET (TFET) device, where the channel is a heterojunction based on 2D semiconducting MoTe2 and SnS2 monolayers [3]. We characterize the electronic structure and the transport properties of the 2D-TFET device by means of density functional theory (DFT) combined with the non-equilibrium Green's function (NEGF) method [4] and with advanced electrostatic solvers, as implemented in the QuantumATK software [5]. We show how the electrical response of the device to electrostatic gates can be tuned by using an asymmetric contact scheme. The latter is analogous to that proposed for graphene-based photodetectors [6], where metals with different work functions have been used to contact the 2D channel. Our large-scale DFT-NEGF device simulations demonstrate that the electrical characteristics of ultra-scaled 2D devices can be engineered by an appropriate choice of the metallic electrodes, and highlight the importance of atomistic device simulations for the optimization of the electrical characteristics of future devices based on non-conventional semiconductors.

[1] G. Fiori et al. Nat. Nanotech. 9, 768 (2014).

[2] https://irds.ieee.org/images/files/pdf/2017/2017IRDS_MM.pdf

[3] A. Szabó, IEEE Electron Device Letters 36, 514 (2015).

[4] M. Brandbyge et al., Phys. Rev. B 65, 165401 (2002).

[5] S. Smidstrup et al., in preparation.

[6] F. Xia et al. Nature nanotechnology 4, 839 (2009).

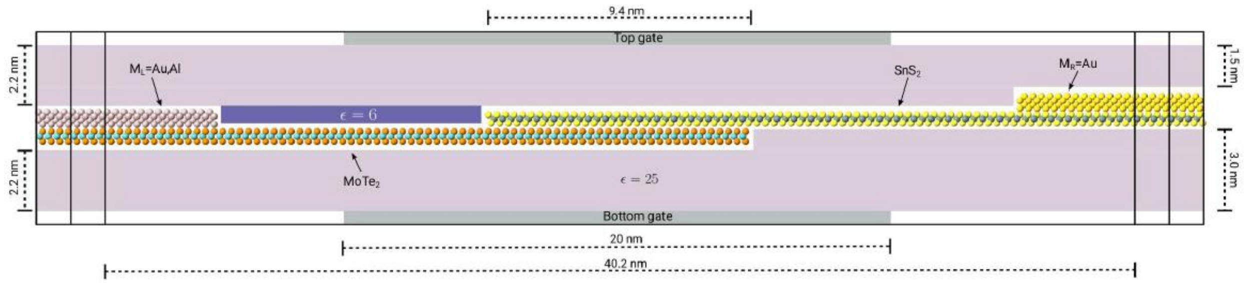

Fig. 1: Structure of the M_L/MoTe2/SnS2/M_R device. Mo, Te, Sn and S atoms are shown in cyan, orange, dark green and yellow. The atoms of the M_L (Au, Al) and M_R (Au) regions are shown in pink and yellow. The metallic gate regions (Top gate, Bottom gate) are shown as grey rectangles. The dielectric regions are shown as dark purple (ϵ = 6) or light purple (ϵ = 25) rectangles.

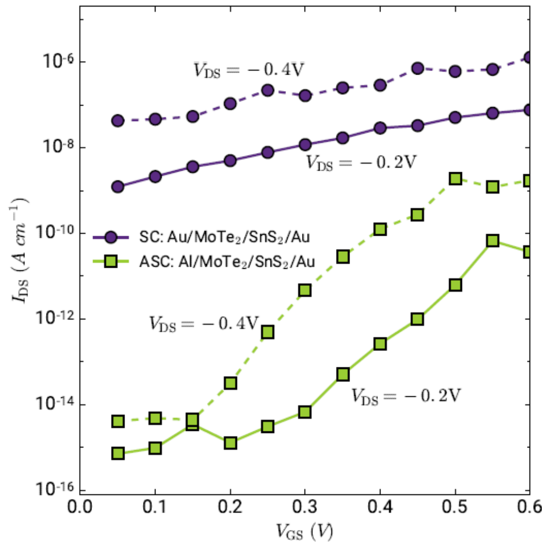

Fig. 2: I_{DS} vs. V_{GS} transconductance curves calculated for the symmetrically-contacted (SC, Au/MoTe2/SnS2/Au) device at V_{DS} = -0.2 V (purple circles, solid line) and V_{DS} = -0.4 V (purple circles, dashed line), and for the asymmetrically-contacted (ASC, Al/MoTe2/SnS2/Au) device at V_{DS} = -0.2 V (green squares, solid line) and V_{DS} = -0.4 V (green squares, dashed line).

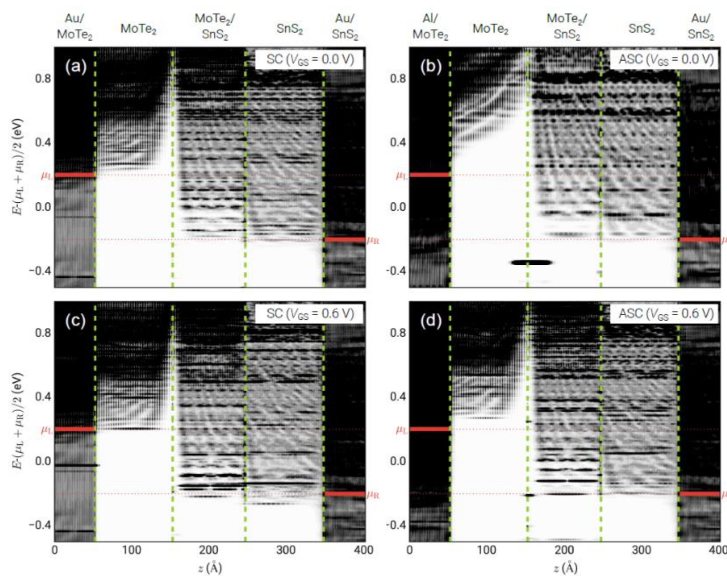

Figure 3: Projected local density of states (PLDOS) along the transport direction for the symmetrically-contacted (SC:Au/MoTe2/SnS2/Au) device at V_{DS} = -0.4V and V_{GS} = 0.0V (a) or at V_{GS} = 0.6V (c). (b,d) Same as (a,c), but for the asymmetrically-contacted (ASC: Al/MoTe₂/SnS₂/Au) device. The red solid lines indicate the position of the left and right chemical potentials. The green dashed lines mark the boundaries of the different device regions.