First-Principles Simulations of 2D Material Heterojunction Tunneling Field-Effect Transistors using QuantumATK

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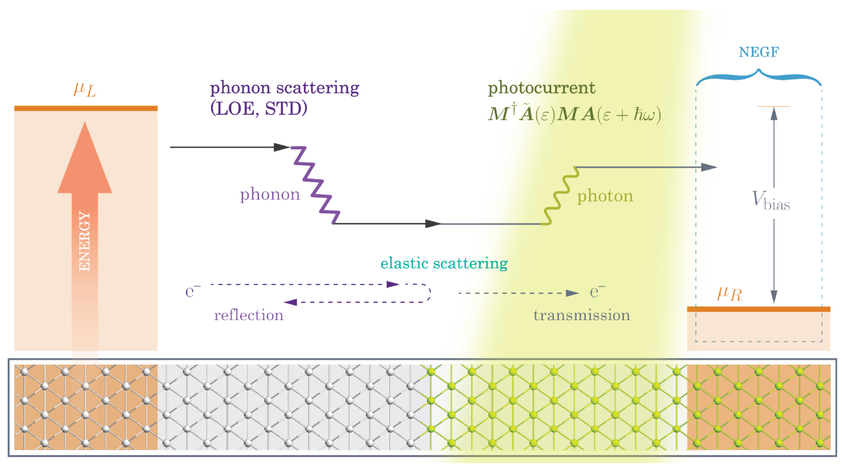
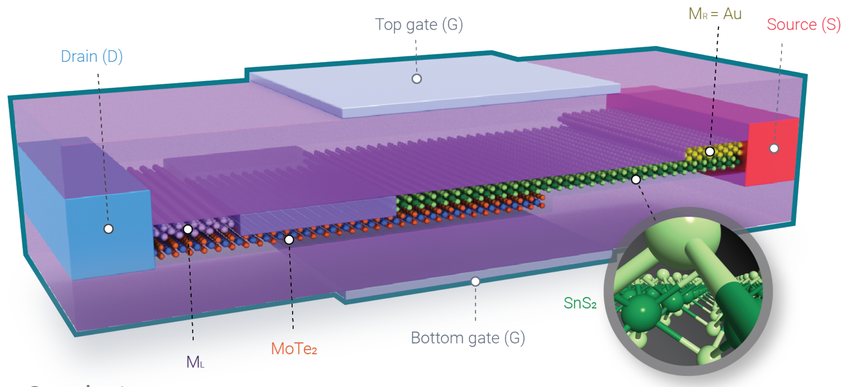
Abstract

Two-dimensional (2D) materials are very attractive for the nanoelectronics industry since they could become the new channel materials of the future nanoelectronics devices and solve the problems related to non-negligible quantization of Si electronic structure upon scaling. Here, we present our group's work on simulating a **2D materials-based heterojunction Tunneling Field-Effect Transistor (TFET)** with **Density Functional Theory (DFT)** and **Non-Equilibrium Green's Functions (NEGF)** methods in the QuantumATK software suite[1,2]. Specifically, we consider a (SC) and asymmetrically-contacted (ASC) TFET where the channel is formed by a heterojunction based on two-dimensional (2D) semiconductors: $MoTe_2|SnS_2$[3]. In the SC device, we use Au for both the source and drain metallic contacts, whereas in the ACS device, we use Al in the drain, in order to have a rather large work function difference between the contacts. Our simulations show how the device trans-conductance of a TFET can be engineered by an appropriate choice of the metallic electrodes. The results also highlight the importance of atomistic device simulations for the optimization of the electrical characteristics of devices based on non-conventional materials.

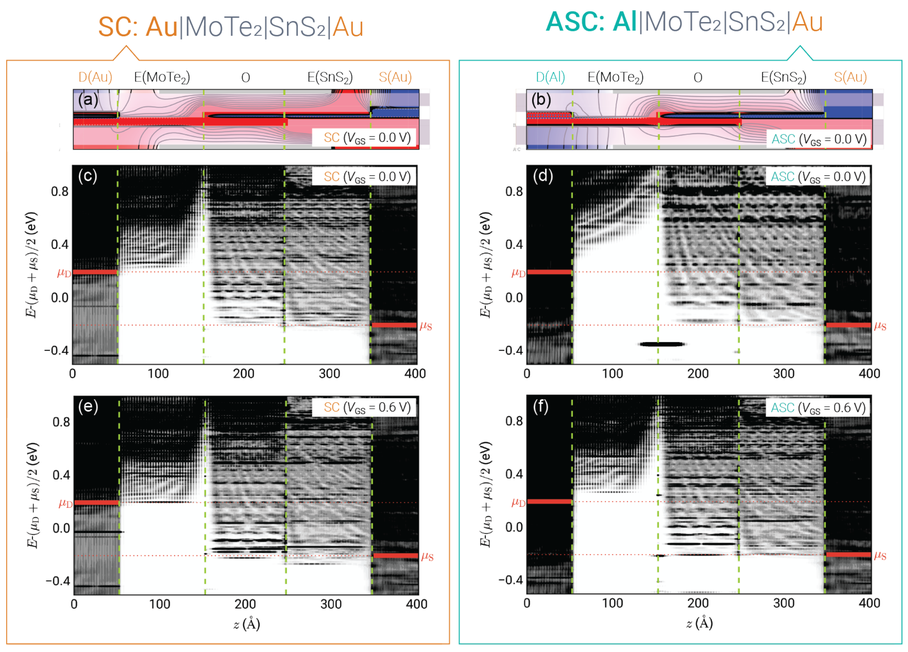


Computational Method: The combination of DFT-LCAO with the NEGF method in QuantumATK, enabling simulations of the electronic structure and electrical characteristics of devices. In the NEGF method, it is possible to include the effect of gate potentials in the selfconsistent solution. Inelastic effects due to phonon or photon scattering can be included through perturbation theory.

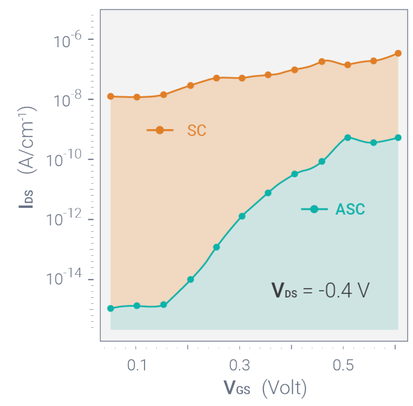


System: 2D-TFET device, where the channel is formed by a $MoTe_2|SnS_2$ heterojunction. We consider two contact schemes:

- SC: Au|$MoTe_2|SnS_2$|Au
- ASC: Al|$MoTe_2|SnS_2$|Au



(a, b): Cut-planes of the Hartree difference potential.
(c, d, e, f): The projected local density of states (PLDOS) along the devices.



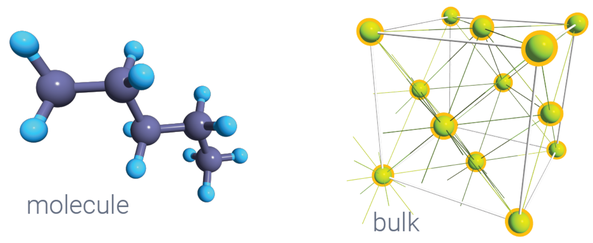
Trans-conductance: Reverse-bias I_{DS}-V_{GS} curves at the drain-source voltage, V_{DS}=-0.4 V.

Conclusions:

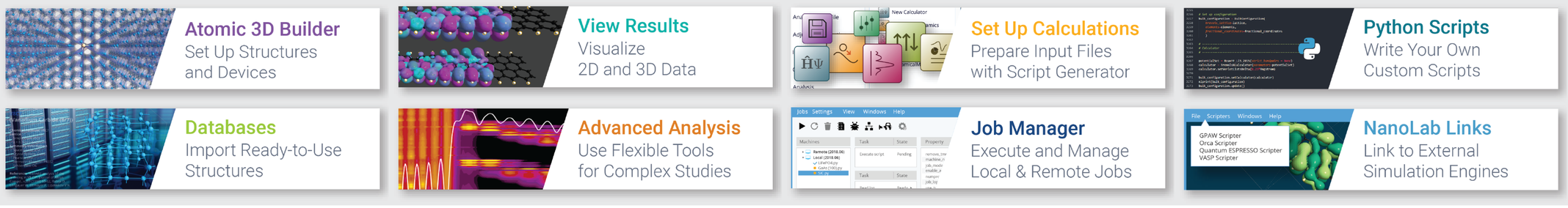
- The drain-source current, I_{DS}, is higher in the SC device than in the ASC device across the entire range of gate-source voltages.
- In the SC device, I_{DS} increases only by a factor of 10, whereas in the ASC device, I_{DS} increases by about six orders of magnitude in the same V_{GS} range.
- The transconductance behavior can be understood from the combined analysis of the Hartree difference potential and of the PLDOS. In the ASC device, the use of two metals with different work functions leads to an additional built-in electric field in the channel region, which affects the device electrostatics and electronic structure.

QuantumATK Platform

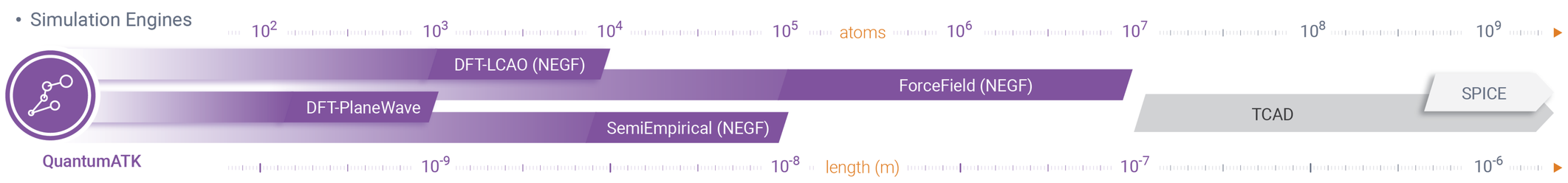
- System Configurations



- NanoLab GUI



- Simulation Engines



References

[1] QuantumATK, version P-2019.03, Synopsys QuantumATK (synopsys.com/silicon/quantumatk.html).
[2] QuantumATK: An integrated platform of electronic and atomic-scale modelling tools, S. Smidstrup, T. Markussen, P. Vancraeyveld, J. Wellendor, J. Schneider, T. Gunst, B. Verstichel, D. Stradi, P. Khomyakov, U. G. Vej-Hansen, M-E. Lee, S. Chill, F. Rasmussen, G. Penazzi, F. Corsetti, A. Ojanperä, K. Jensen, M. Palsgaard, U. Martinez, A. Blom, M. Brandbyge, K. Stokbro, arXiv:1905.02794v1 [cond-mat.mtrl-sci] (2019).
[3] G. Fiori, F. Bonaccorso, G. Iannaccone, T. Palacios, D. Neumaier, A. Seabaugh, S. K. Banerjee, and L. Colombo, Nat. Nanotech. 9, 768 (2014).