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 for 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. Specifically, we consider a (SC) and asymmetrically-contacted (ASC) TFET where the channel is formed by a heterojunction based on two-dimensional (2D) semiconductors: MoTe2/SnS2. In the SC device, we use Au for both the source and drain metallic contacts, whereas in the ASC 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 enables 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 self-consistent solution, relaxes the effects due to phonon or photon scattering can be included through perturbation theory.

System: 2D-TFET device, where the channel is formed by a MoTe2/SnS2 heterojunction. We consider two contact schemes: SC: Au/MoTe2/SnS2/Au

ASC: Al/MoTe2/SnS2/Au

Conclusions:
The on-source current, Ios, is higher in the SC device than in the ASC device across the entire range of gate-source voltages, in the SC device, Ios increases only by a factor of 10, whereas in the ASC device, Itos increases by about six orders of magnitude in the same Vgs range.
The transconducance behavior, can be understood from the combined analysis of the barrier height potential and of the PLOBS. 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
- Atomic 3D Builder
- Set Up Structures and Devices
- Databases
- View Results
- Advanced Analysis
- Use Potted Tests for Complex Studies
- View 2D and 3D Data
- Set Up Calculations
- Prepare Input File with Script Generator
- NanoLab Links
- Python Scripts
- Write Your Own Custom Scripts

References

[1] QuantumATK. version 7.2.0.03, Synopsys QuantumATK (synopsys.com/silicon/quantumatk.html)