Atomistic quantum mechanical simulation of transient currents through nano-structures and multiscale simulation of junctionless transistor

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BACKGROUND

As the feature size of electronic devices inches toward 10 nanometers, simulations including quantum effects and atomistic details are inevitable. Two of many important issues need to be addressed. As the clock speed increases, dynamic response of nanometer-scale molecular electronic devices becomes important. This requires the use of quantum mechanics to ensure the proper treatment of transient currents and response. In the aspect of integrated circuit designing, the conventional compact models are based on classical continuum models, and thus no longer applicable for sub-10nm devices. Hence, it is necessary to develop a new multiscale method that bridges the quantum mechanical simulation and the industrial modeling tools such as the compact models.

ATOMISTIC QUANTUM MECHANICAL SIMULATION OF TRANSIENT CURRENT

To simulate the transient electrical currents through a molecular device (D) coupled with two electrodes (L and R), we employ the rigorous time-dependent density functional theory (TDDFT) that we developed previously.[1] Our theory uses a closed equation of motion (EOM) for the reduced single-electron density matrix of the molecular device D, σ_D, as follows:

$$i\dot{\sigma}_D = [h_D[r,t;\rho_D(r,t),\sigma_D] - i\sum_{\alpha=L,R} Q_\alpha[r,t;\rho_D(r,t)]$$

This is the first-principles Liouville-von Neumann equation for the reduced single-electron density matrix. And the transient current J trough the left (right) electrode is obtained via the trace of corresponding dissipative term $Q_L(Q_R)$:

$$J(t) = -Tr[Q(t)]$$

For a CNT-based conductor shown in **Fig. 1**, we calculated the dynamic admittance and time-dependent charge distribution as shown in **Fig. 2**. [2] It is found that the electrical response of these two-terminal molecular devices can be mapped onto an equivalent classical electric circuit. This result is confirmed by studying the electric response of simple two-site model and can be generalized to other two-terminal molecular electronic devices.

MULTISCALE SIMULATION OF JUNCTIONLESS TRANSISTOR

To develop an accurate as well as efficient method for simulating nanoscale electronic devices, we combine quantum mechanics and electromagnetics together and develop a novel hybrid QM/EM method.[3] The system of interest is partitioned into an active scattering region which is described quantum mechanically and the rest includes interconnects and semiconductor matrices where a classical description is sufficiently accurate. In our approach, the QM region is simulated using the combined DFTB + NEGF method while the outer EM region is treated with semi-classical drift-diffusion model. QM and EM calculations are linked by means of boundary condition between the two regions and are solved iteratively until self-consistency is achieved. The QM/EM provides a seamless bridge between atomistic quantum mechanical simulation and the compact model.

We apply the QM/EM method to calculate the I-V curves for a junctionless transistor as depicted in **Fig. 3**. The calculation results are consistent with the measurement.

CONCLUSION

The first-principles Liouville-von Neumann equation is based on the equation of motion for the reduced single-electron density matrix, and can thus be solved for realistic nanoscopic devices. We have employed it to simulate the transient electrical response through a series of systems including a CNT-based electronic device. Important information about the ultrafast processes in such a device is obtained. We have also developed a multiscale QM/EM method for electronic device simulation. The method includes both macroscopic drift-diffusion current model and quantum tunnelling model which are solved together in a self-consistent way. The QM/EM method may constitute as an important component of next generation electronic design automation (EDA) tools.

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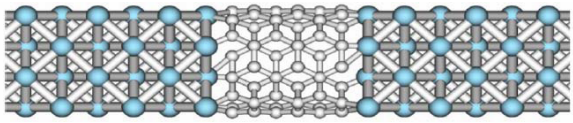

Fig. 1. Prototype used for explicit QM calculations of a CNT-based conductor. The (5,5) CNT device with aluminum as electrodes.

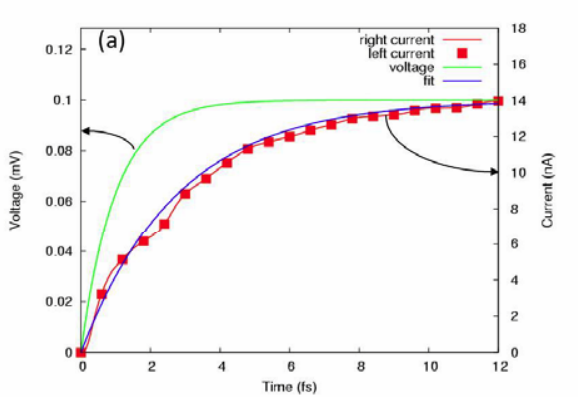

Fig. 2a. Transient current (red line and squares) and applied bias voltage (green line) for the Al–CNT–Al system. The bias voltage is turned on exponentially, $V_b = V_0(1 - e^{-t/a})$ with $V_0 = 0.1$ mV and a time constant a = 1 fs. The blue solid line is a fit to the transient current.

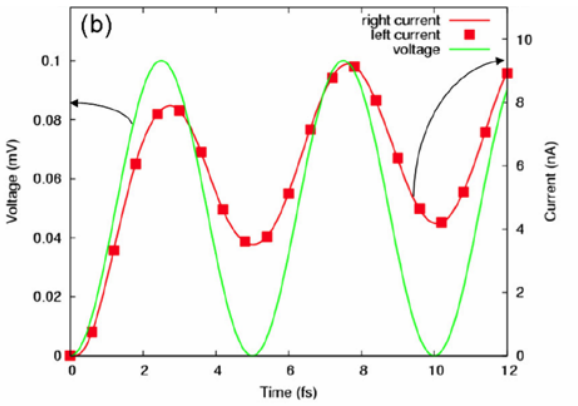

Fig. 2b. Transient current (red line and squares) and applied bias voltage (green line) for the Al–CNT–Al system. The bias voltage is sinusoidal with a period of 5 fs. The red line is for current from the right electrode, and squares are current from the left electrode.

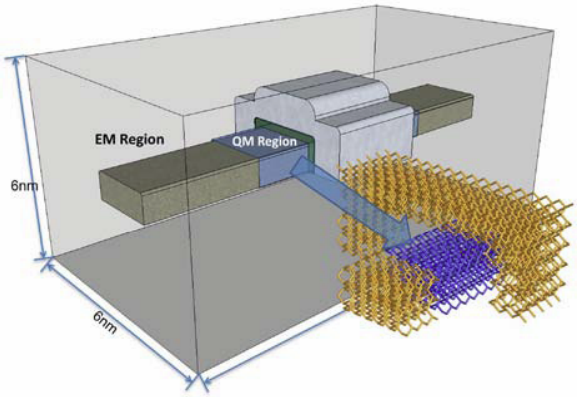

Fig. 3. QM/EM simulation model of a junctionless transisitor. QM region is where the atomistic quantum mechanical simulation is carried out.