

# Transport Properties of C<sub>3</sub>N Nanoribbon-Based Nanoscale Transistors

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**Abstract**—In this paper, the transport properties of field-effect transistors based on armchair C<sub>3</sub>N nanoribbon saturated by hydrogen are theoretically analyzed through a multiscale simulation procedure from first-principles computation to the tight binding analysis. Density Functional Theory(DFT) for the electronic structure, maximally localized Wannier functions(MLWF) for the tight-binding(TB) hamiltonian, and nonequilibrium Green's function(NEGF) formalism for the transport properties. The band structure, transmission coefficient and the  $I$ - $V$  curves are calculated. Simulation results show that gate length has a great effect on the transport properties of transistors based on armchair C<sub>3</sub>N.

**Keywords**—C<sub>3</sub>N nanoribbons; transport properties; electron devices; nanoscale transistor; multiscale simulation flow

## I. INTRODUCTION

When characteristic dimensions of transistors are going below 10 nm, fundamental limitations are emerging both in terms of manufacturing costs and device performance. To sustain Moore's law, it is essential that the transistor material and the manufacturing process should be changed. For the transistor material, using two-dimensional (2D) systems as conduction channels is definitely one of the most exciting opportunities [1]. Recently, C<sub>3</sub>N, one graphene-like material, has been investigated. The authors have put forward the hypothesis that C<sub>3</sub>N could be attractive for device applications such as optoelectronics [2]. Only an accurate simulation of a complete device can testified this hypothesis and satisfy experimental interest in the novel 2D materials. This task is not straightforward, however, the simulation of a device requires a preliminary characterization of the material.

In this paper, A multiscale approach based on DFT method, MLWF interpolation and NEGF formalism is performed to study the transport properties of nanoscale transistors with different channel width. All the computations are accomplished in three open packages: *VASP* for *ab initio* calculations [3], *Wannier90* for MLWF interpolation [4] and *NanoTCAD ViDES* for computing transport properties [5].

## II. DEVICE STRUCTURE AND SIMULATION SCHEME

### A. Device Structure

As shown in Fig. 1, the model of double-gate field-effect transistor is established. The channel lengths of the transistors

are 8 nm, 10 nm and 12 nm respectively, and the width is 1 nm, with transport of z-direction. The source and drain regions where the bias voltage is applied and current are semi-infinite, respectively. The gates are as long as the channel and are treated as ideal metal. Two oxide layers made of SiO<sub>2</sub> are 0.5 nm thick wrap around the channel.

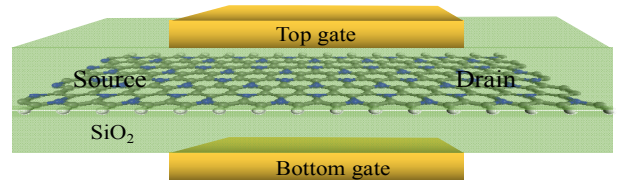


Fig. 1. Double-gate metal-oxide-semiconductor FETs based on C<sub>3</sub>N Nanoribbon channel.

### B. Simulation Scheme

Taking advantage of the high precision of DFT method in computing electronic structure and the high efficiency of TB in numerical simulation, we adopted a multiscale simulation scheme to analyse the transport properties of the transistors.

DFT method for obtaining the band structure and wave functions of the C<sub>3</sub>N nanoribbon supercell [6]. We chose four valence bands and four conduction bands near the Fermi level contribute to the transport mostly and the related wave functions as the inputs for MLWF interpolation. For a set of  $N$  Bloch bands  $\psi_{nk}$ , a set of  $N$  wannier functions  $w_{nR}$  are constructed as

$$|w_{nR}\rangle = \frac{V}{(2\pi)^3} \int_{BZ} \left[ \sum_{m=1}^N U_{mn}^{(k)} |\psi_{mk}\rangle \right] e^{-i\mathbf{k}\cdot\mathbf{R}} d\mathbf{k} \quad (1)$$

where  $V$  is a real-space unit cell volume of the crystal,  $k$  is the wave vector, BZ is the Brillouin zone over which the integral performed,  $\mathbf{R}$  is Bravais lattice vector,  $n$  is the band index, and  $U^{(k)}$  is a unitary matrix. By optimizing the  $U^k$ , the MLWFs Hamiltonian retaining full first principles accuracy for the relevant electronic bands will be obtained.

We exploit the NEGF formalism to compute the currents in a complete device. The Green's function is computed as

$$G(E) = [ES - H - \Sigma_s - \Sigma_d]^{-1} \quad (2)$$

where  $E$  is the energy,  $S$  is the identity matrix,  $H$  is the Hamiltonian comes from the wannier functions interpolation.

$\Sigma_D$  and  $\Sigma_S$  are the self-energy of the drain and source contacts, respectively. The relationship between Hamiltonian and self-energy is showed in Fig. 2.

The transmission coefficient  $T(E)$  is computed as

$$T(E) = -Tr[(\Sigma_S - \Sigma_S^\dagger)G(\Sigma_D - \Sigma_D^\dagger)G^\dagger] \quad (3)$$

where  $Tr$  is the trace operator,  $\Sigma_S^\dagger$ ,  $\Sigma_D^\dagger$  and  $G^\dagger$  is the conjugate transpose matrix of  $\Sigma_S$ ,  $\Sigma_D$  and  $G$  respectively.

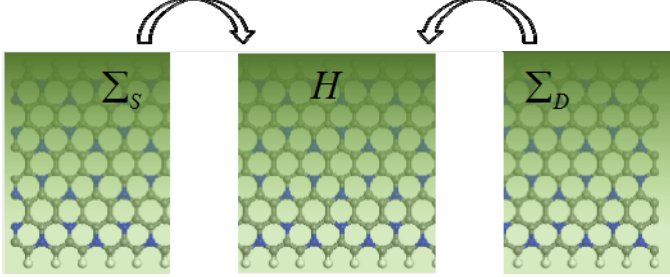


Fig. 2. The NEGF method: The device is defined by the tight-binding Hamiltonian  $H$ , which is combined with the source and drain by the self-energy  $\Sigma_S$  and  $\Sigma_D$ .

Hence, the current flowing through the device can be computed as

$$I = \frac{2q}{h} \int_{-\infty}^{+\infty} dE T(E) [f(E - E_{F_S}) - f(E - E_{F_D})] \quad (4)$$

where  $q$  is the electron charge,  $h$  is Planck's constant,  $E_{F_S}$  and  $E_{F_D}$  is the fermi level of the source and drain, respectively. Function  $f(E)$  is Fermi distribution function.

### III. SIMULATION RESULT

The energy bands computed from DFT method and the results from MLWFs interpolation is compared in Fig. 3. The bands calculated from DFT method described in blue lines are insured correct, while the results from MLWF are depicted in empty circles. It can be seen that they are perfect fitted. This explains the tight-binding Hamiltonian from the Wannier interpolation has high accuracy to represent the device system. Then the Hamiltonian can be sent to the *NanoTCAD ViDES*.

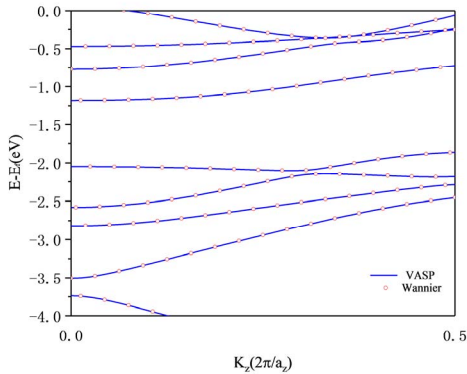


Fig. 3. Empty circles: results from Wannier interpolations. Blue lines: results from DFT method calculation.

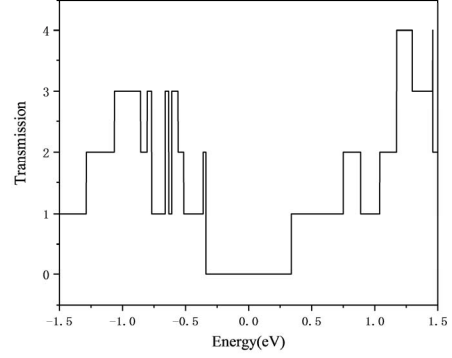


Fig. 4. The transmission coefficient calculated by NEGF method.

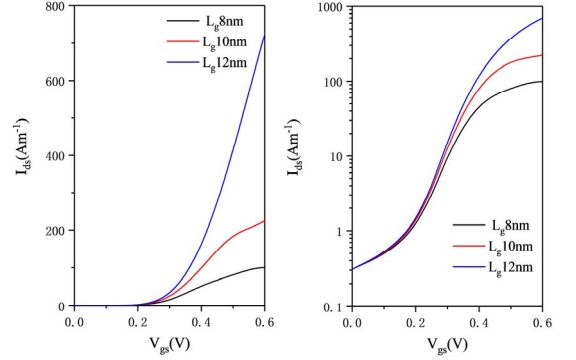


Fig. 5.  $I_{ds} - V_{gs}$  curve in left is linear and the right is semi-logarithmic scale for  $C_3N$  transistors with  $L_g=8$  nm, (black line),  $L_g=10$  nm (red line),  $L_g=12$  nm (blue line). All simulations bias voltages  $q\phi = 0.1$  V.

Fig. 4 shows the transmission coefficient, and the width of zero value is 0.67 meet with the indirect bandgap calculated by DFT method, explaining our method to simulate the transport properties of  $C_3N$  nanoribbon based transistors is precise. We performed an investigation along the device parameter space, we have computed the  $I - V$  characteristics for different gate lengths. Fig. 5 shows the changes of currents according to the lengths of the gate. The maximum current of the transistor with  $L_g=12$  nm is almost 4 times than the other two curves. As a consequence, from designing and manufacturing point of view, while the control of the gate lengths is required.

### IV. CONCLUSION

In this paper, we used a multiscale simulation approach to study the transport properties of the transistors with different gates length based on armchair  $C_3N$  nanoribbon which saturated by hydrogen. Simulation results showed that to design a well gate-controlled transistor, appropriate gate length is essential.

### ACKNOWLEDGMENT

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