

# Nanoelectronic Device Simulation Using Extended Hückel Theory (EHT) and NEGF

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## ABSTRACT

Nanoelectronic devices can be, in one way, characterized by the large surface/volume ratio in addition to the central role of quantum effects. This paper describes a computationally efficient way of obtaining the bandstructure of the intrinsic device including the interface with metal contacts using the extended Hückel theory (EHT). Carrier quantum transport is then computed by NEGF (non-equilibrium Green's function). GNR-FETs (graphene-nanoribbon FET) are simulated using this approach as an application example.

## 1 INTRODUCTION

Recent experimental work on GNR-FETs [1] reconfirms the critical role of Schottky contact between the semiconductive channel and metal source/drain (S/D) regions in the transistor operation for carbon crystal, e.g. CNT (carbon nanotubes) and GNR, based field-effect devices. It is actually a common fact that all nanoelectronic devices are characterized by a large surface-volume ratio and the correct modeling of the material interface becomes an essential part of device simulation.

## 2 Principles of EHT Method

EHT can be characterized as one of LCAO (linear combination of atomic orbitals) methods in solving Schrödinger equation for a system to obtain its electronic structure: either energy levels for molecules or bandstructure of  $E(\mathbf{k})$  for crystals. Different from orthogonal TB method, the basis functions in EHT are directly tied to the atomic orbitals with a more localized treatment, the Slater-type orbitals (STO) [3] as follows,

$$\phi_{nlm}(\mathbf{r}) = \sigma r^{n-1} e^{-\zeta r} Y_{lm}(\theta, \varphi) (= \text{STO}) \quad (1)$$

where spherical coordinates  $r, \theta, \varphi$  have been used for  $\mathbf{r}$ , and  $n (= 1, 2, \dots), l (= 0, 1, \dots, n-1), m (= -l, -l+1, \dots, 0, 1, \dots, l-1, l)$  are principal, angular momentum, and magnetic quantum numbers, respectively, and  $Y_{lm}(\theta, \varphi)$  is the real-valued spherical harmonics.  $\zeta$  is called the orbital exponent and is related to the effective nuclear charge (the nuclear charge partially shielded by electrons in the core of an atom).  $\sigma$  is the normalization constant and is obtained from

$$\sigma^2 \int_0^\infty (r^{n-1} e^{-\zeta r})^2 r^2 dr = 1 \implies \sigma = \frac{(2\zeta)^{n+1/2}}{\sqrt{(2n)!}} \quad (2)$$

With the above AOs, we consider first molecules or a primitive cell in crystals. The complete set of basis functions are

$$\begin{aligned} & [\phi_1(\mathbf{r}) \phi_2(\mathbf{r}) \cdots \phi_N(\mathbf{r})]^T = \\ & [\phi_{11} \phi_{21} \cdots \phi_{N_{\text{ao}}1} \phi_{12} \cdots \phi_{N_{\text{ao}}2} \cdots \phi_{1N_{\text{at}}} \cdots \phi_{N_{\text{ao}}N_{\text{at}}}]^T \end{aligned} \quad (3)$$

where we have omitted the explicit function argument  $\mathbf{r}$  on the right-hand side,  $N = N_{\text{ao}} \times N_{\text{at}}$  with  $N_{\text{ao}}$  the number of AOs associated with each atom (assumed the same for all atoms) and  $N_{\text{at}}$  that of atoms (in the molecule or cell).

$$\phi_{ij}(\mathbf{r}) = \text{STO}_i(\mathbf{r} - \mathbf{d}_j), \quad i = 1, \dots, N_{\text{ao}}, j = 1, \dots, N_{\text{at}} \quad (4)$$

where  $\mathbf{d}_j$  is the displacement of atom  $j$  relative to atom 1 ( $\mathbf{d}_1 = \mathbf{0}$ ) in the cell.

The elements of Hamiltonian  $H$  are calculated in principle from

$$H_{ij} = \int \phi_i^* H \phi_j d\mathbf{r} \quad (5)$$

where  $H$  is the Hamiltonian for the entire system. In practice, EHT uses simple formulas to evaluate Hamiltonian matrix elements in the following way:

$$\begin{aligned} H_{ii} &= \varepsilon_i + U_{i,\text{shift}} - qV_i \\ H_{ij} &= \frac{1}{2} S_{ij} [K_{\text{EHT}}(\varepsilon_i + \varepsilon_j) + U_{i,\text{shift}} + U_{j,\text{shift}} \\ &\quad - q(V_i + V_j)], \quad i \neq j \end{aligned} \quad (6)$$

The above expression for  $H_{ij}$  is named after Wolfsberg-Helmholtz, where  $K_{\text{EHT}}$  is a fitting parameter of typical value of 1.75 for molecules, 2.3 for solids, and 2.8 for 2D graphene sheets [2].

Special discussion is needed for formula of  $H_{ii}$  (6).  $\varepsilon_i$  is the on-site energy (also called the valence state ionization potential, or VSIP) and is an empirical parameter listed, e.g., in [4] for all elements in the Periodic Table. Since EHT-related parameters may be obtained from different energy reference setting (e.g., the Fermi-level for transitional metals is set to -10 eV and the top of valence band for semiconductors is set to -13 eV), it is important to make sure that the vacuum level is set to the same level for all the atoms in the system, thus arising the parameter  $U_{i,\text{shift}}$  in, where all  $U$ s corresponding to a single atom have the same value. In addition, the potential at each atom is a variable determined from solving Poisson's equation, so it may need to be accounted for

in rigorous calculations. A slightly different recipe for obtaining  $H_{ij}$  can be found in [2].

Thus completed the description of the EHT method.

### 3 NEGF Simulation of Quantum Transport

NEGF is used in simulation of carrier quantum transport in the system with the open boundary conditions. The surface Green functions, which characterize the contacts to the system are obtained by an iteration scheme. The Green's function in the device region is calculated by

$$G^R = [(E + i\eta)S - H(U_H) - \Sigma]^{-1} \text{ with } \eta \rightarrow 0^+ \quad (8)$$

where  $G^R$  is the retarded Green's function,  $H$  is the Hamiltonian of the system with closed BCs, whose eigenenergy can be labeled  $\epsilon_n$  ( $n = 1, \dots$ );  $E$  is a given energy which is continuous but not equal to  $\epsilon_n$ ;  $U_H$  is the external potential energy (called Hartree potential) and will affect  $H$  through (6-7) (hence  $H$  as function of  $U_H$  in the above expression), and  $\Sigma$  is the self-energy characterizing the semi-infinite contact regions.  $U_H$  depends on the carrier concentration profile and is solved from the Poisson's equation. So both Schrödinger and Poisson's equations have to be solved self-consistently.

### 4 Simulation Example

As an example of applying EHT-NEGF method for device simulation, we have investigated how the width of an armchair GNR (aGNR) affects the bandgap in the electronic structure. In our simulation, it is found that the bond length is weakly dependent on the number of carbons across the ribbon width ( $N_a$  in Fig. 2, and the C-C bonds in the channel direction at two edges of the

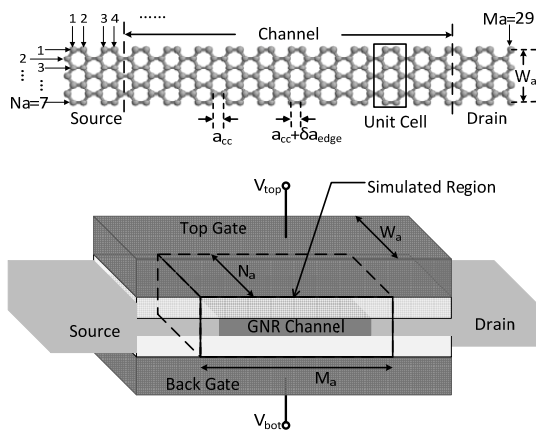


Figure 1: Schematics of GNR-FET. (a) The armchair GNR structure with  $N_a = 7$  and  $M_a = 29$  is chosen for the simulated region; (b) The DG structure of the simulated device. The Fermi level is set to  $-12.3$  eV at drain and source while that for GNR channel  $-13.0$  eV [6], and  $t_{ox} = 0.5$  nm.

ribbon are shortened by 3.4% to reflect the effects of

the termination of graphene edge. The results from our simulation (Fig. 5) are similar to those from the TB and first-principles calculations. Unlike TB, EHT does not need structure-dependent fitting parameters, especially for systems whose physical properties are strongly affected by the geometry, and the computational cost is acceptable. Fig. 2 shows how bandgaps at different  $N_a$  vary with the bond length at edges. Since the electronic structure of armchair GNR has a quantized width-dependence, GNR with  $N_a = 3p + 1$  (where  $p$  is a positive integer) will provide good performance. Fig. 2 shows the double-gate (DG) GNR-FET in our simulation with  $N_a = 7$  and  $M_a = 29$ . A comparison of transport characteristics simulated using the EHT-based and TB-based NEGF is shown in Fig. 3.

Bond length relaxation of GNR is taken into account in the EHT calculation, and has a significant influence on the transport. Fig. 4 shows the output characteristics simulated with independent gate operation. A stronger short-channel effect in EHT simulation is observed, compared to TB, as well as an exceedingly high drain current in the saturation region with  $a_{cc} = 1.44$  Å.

### 5 Conclusions

Even though both TB and EHT are semi-empirical, i.e., depending on the fitting parameters to some extent, in nature, the latter has more direct link to the atomic orbitals of the constitutive atoms. This feature of EHT can help identify the charge transfer for the chemical bonds at the material interface and has significant applications such as determining the dipole at the interface.

### 6 Acknowledgement

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