Introduction of Wannier function into TOMBO

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Abstract

Following Moore's law, the number of transistors on the integrated circuits doubles approximately every two years. However, the size of transistors cannot be infinitive small, because of the quantum effects. The ultimate size of the transistors is molecule. Therefore, the effective method to simulate the electron transport properties through the molecules plays an important role in understanding and design of molecular transistors.

A typical molecular transistor is depicted in Fig. 1, where the molecule (benzene-dithiol) is connected to two semi-infinitive gold leads.

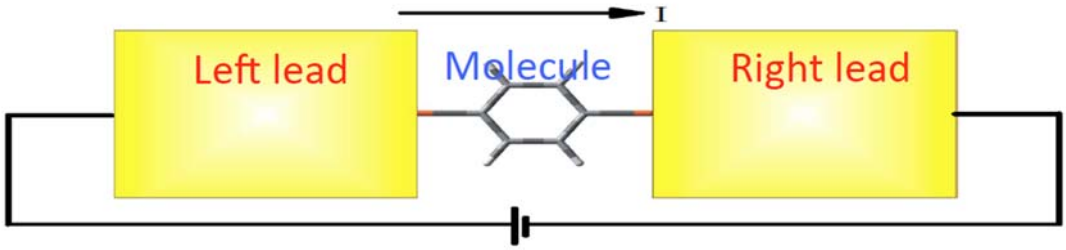

Fig. 1. Benzene-dithiol connecting with two Au leads.

Compared with the original algorithm used in traditional DFT calculations, it is hard to apply the DFT simulation directly to this new system. Because

1) Two semi-infinitive leads make the whole system infinitive,
2) The whole system is not periodic, and
3) If the bias is applied, the system is non-equilibrium.

In traditional calculations, it is impossible to deal with an infinitive system without translation invariance and the simulated system should be in equilibrium (as shown in Fig.2, left panel). To self-consistently calculate the transport properties, for example, the current flows through the molecules, we have to introduce the non-equilibrium Green's function (NEGS) into TOMBO. By using NEGF, two leads are represented by the self-energy terms, whose dimension is same as the dimension of the molecule. If the bias is applied, the redistribution of the non-equilibrium electron can be calculated by Green functions (shown in Fig. 2, right panel).

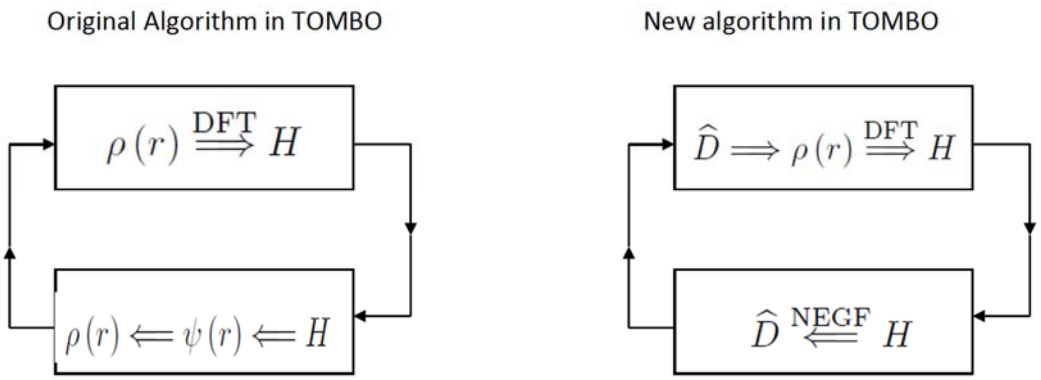

Fig. 2. The comparison of algorithm used in traditional DFT calculation (left) and the electron transport properties simulations (right).

To calculate the self-energy terms, the interactions between the leads and the molecule should be extracted. The whole system should be divided into three parts, left lead, right lead, and the molecules. The system is solved self-consistently until the criteria are satisfied. After this procedure, the I-V curves and the transmission coefficients can be computed numerically.

However, the mixed basis (the plane waves and the atomic orbitals) sets are used in TOMBO, and it is impossible to divide the whole system by using the plane waves due to its delocalization. To realize the simulations, Wannier function should be used.

Since the undetermined phase factor, different equivalent Wannier function can be defined. In our calculations, the so-called maximum localized Wannier function (MLWF) is used. The reason we choose MLWF because:

1) This definition is independent on the basis set used in calculations,
2) The algorithm is realized by library Wannier90, and
3) Only the interface between Wannier90 and TOMBO is required to realize the calculations.

After introduction MLWF, the calculation of different self-energy terms are possible and we can study the electron transport based on the self-consistent DFT simulations.