

# Atomic-scale modelling of electron transport across metal-organic interfaces

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## ABSTRACT

*We study the atomic and electronic structure of a metal-organic interface using Density Functional Theory combined with Non-Equilibrium Greens Functions (DFT-NEGF)[2]. We calculate the I-V characteristics of the interface and find strong rectification. The electro-static potential shows the formation of a Schottky barrier contact, and we present a new model for transport across an organic semiconductor Schottky barrier which can rationalize the simulation data.*

## INTRODUCTION

The understanding of electron transport across the metal-organic interface is important for development of efficient charge injection into organic devices[1]. The topic of this paper is to understand the charge injection at the atomic-scale and the non-linear bias dependence of the associated contact resistance. The system investigated is a gold-pentacene organic crystal interface. The pentacene crystal is an important organic material for electronics, due to its high hole mobility, and the gold-pentacene interface is one of the most well studied systems both theoretically and experimentally[4].

## SIMULATION

The simulation cell is illustrated in Fig. 1a and 1b. The structure is a so-called two-probe geometry, consisting of a central region connected with semi-infinite left and right electrodes. Fig. 1c shows the local density of states at the interface. The gold electrode has metallic bands, while the organic semiconductor has four narrow bands in the energy range -2, 2 eV. The HOMO band shows Fermi-level pinning at the interface, and this gives rise to the formation of a Schottky barrier.

Fig. 2 shows the calculated I-V characteristics. For the calculation we used a DFT-NEGF approach as implemented in the ATK package[2].

The simulation shows a strong rectification behavior, in agreement with experimental data. The rectification is related to a bias dependence of the Schottky barrier, as shown in Fig. 3. The rectification is much stronger than predicted by conventional inorganic semiconductor Schottky barrier theory. Fig. 4 illustrates that the organic semiconductor has more narrow bands than the inorganic semiconductor, and this gives rise to an additional contact resistance due to the absence of electronic states in the band bending region.

## CONCLUSION

We show that electron transport across a metal-organic interface is dominated by a Schottky barrier. The transport across the barrier is thermally activated, but differs from thermionic emission in an organic semiconductor, since the electrons need to tunnel through the band-bending region, as illustrated in Fig. 4. The model can rationalize recent experiments[4] for the I-V characteristics of the gold-pentacene interface.

## ACKNOWLEDGEMENT

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## REFERENCES

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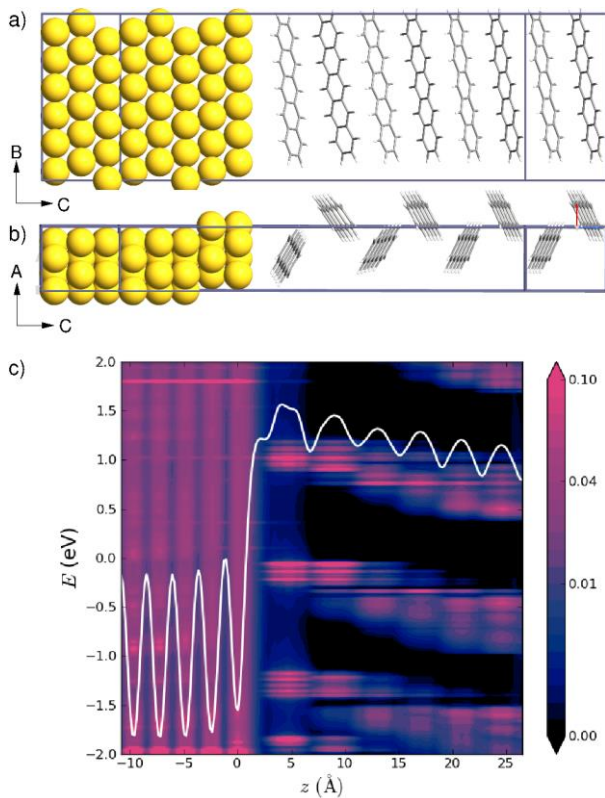


Fig. 1. Side views of a) the B-C and b) the A-C planes of the Au(111)-pentacene interface. The structure is relaxed such that forces are smaller than 0.01 eV/Å. c) Contour plot of the Local Density Of States (LDOS) together with the electrostatic potential (white line) along the z direction. Energy is relative to the electrode Fermi levels and LDOS and the potential is averaged over the x- y directions.

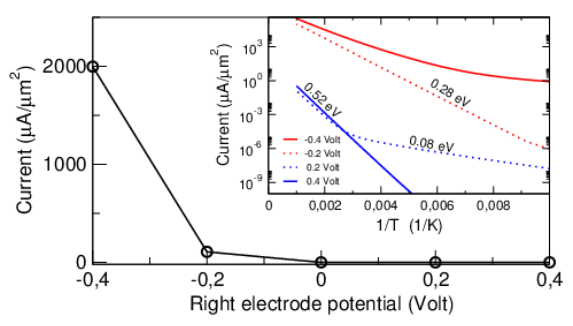


Fig. 2. Current-voltage characteristics of the gold-pentacene interface. Inset shows the temperature dependence of the current at each bias voltage. The temperature dependence shows activated transport, and the height of the activation barrier is indicated for each linear segment.

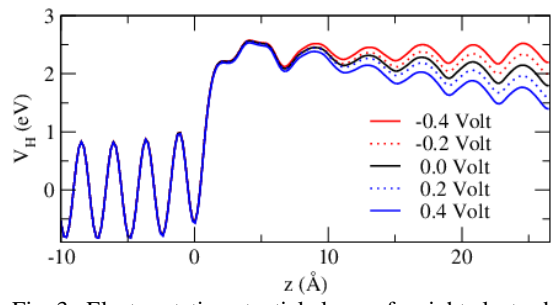


Fig. 3. Electro-static potential along z for right electrode voltages -0.4, -0.2, 0.0, 0.2, 0.4 Volt.

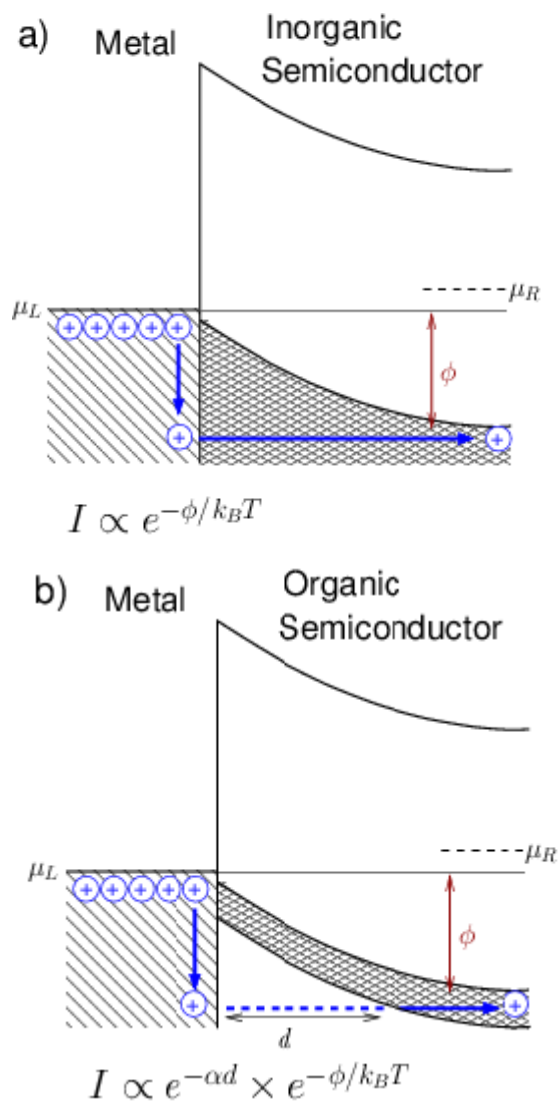


Fig. 4. Band diagram for hole transport across a Schottky barrier at a) Metal-Inorganic Semiconductor interface and b) Metal-Organic Semiconductor interface. The narrow organic crystal bands give rise to tunneling in the band-bending region of the organic semiconductor, reducing the current exponentially.