

## Hybrid-basis modeling of electron transport through molecules on Silicon

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Following considerable recent progress in experimental techniques and theoretical modeling of molecular electronics, the promise of molecular devices has attracted the interest of a lot of physicists, chemists, and engineers towards electron transport in such nanoscale systems. The conducting properties of molecular devices have been theoretically studied by using both first-principles and semi-empirical methods. Most of the ab-initio calculations give accurate electronic structure of isolated molecules; however, transport properties of molecules require an accurate description of the molecule and its interface with the contact under non-equilibrium conditions. Usually the localized basis-sets that describe molecules very well are not efficient in characterizing bulk properties of the contacts, although the latter are quite important for determining the functionality of a device. This becomes particularly important for Si contacts with nontrivial modeling challenges such as its band-edge, surface reconstruction, and surface states. Semi-empirical calculations like Extended Huckel Theory (EHT) or effective mass method are typically better equipped to modeling both the bulk and the surface physics of contacts.

In this work, we develop a formalism to couple two different basis functions in order to accurately model both molecules and contacts under non-equilibrium condition. As an example, we use EHT parameters optimized to describe bulk silicon, and couple it with an ab-initio basis set, 6-31g(d), to simulate the contact surface atoms and the molecules grown on silicon. Such a coupling is achieved by matching the surface green's function in real space in both basis sets. Moreover, we use this hybrid-basis formalism to couple the contacts with a density-functional treatment of the molecule to simulate scanning tunneling spectroscopy (STS) measurements of C60 on a Si substrate as shown in Figure1. Our simulated conductance-voltage curves can be used to explain the different STS results observed experimentally due to the different types of bonding between C60 and Silicon<sup>1</sup>. As a final application of our hybrid-basis modeling technique, we describe STM measurements of organic molecules grown on silicon. Our simulations exhibit a prominent negative-differential resistance (NDR) in such molecular I-Vs due to the interaction between the molecular levels and the silicon band-edge. We are able to use these results to qualitatively interpret experimental observations of room-temperature negative differential resistance<sup>2</sup>.

### References:

1. X. Yao et al. "The bonding nature of individual C60 molecules to Si(100) Surface" *Appl. Phys. A*, 66, S107, 1998.
2. N. Guisinger et al. "Room Temperature Negative Differential Resistance through Individual Organic Molecules on Silicon Surfaces" *Nano Lett.* 2003.

**Si(100)-2x1**      **C60**      **STM**

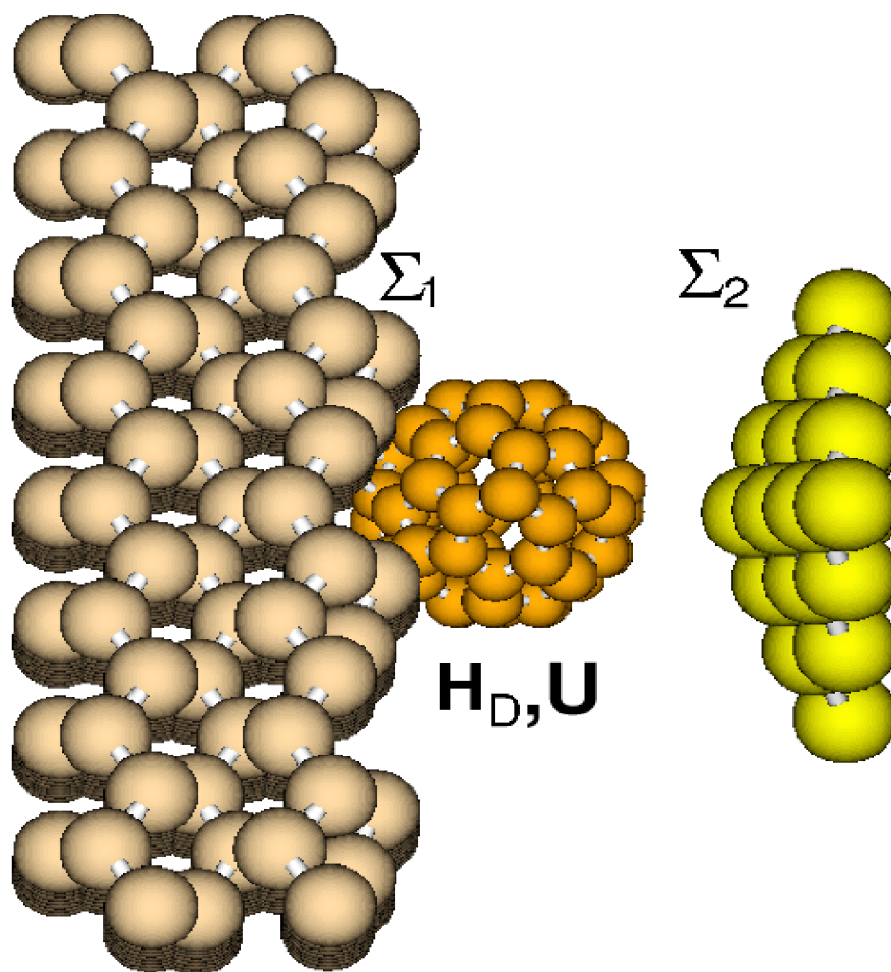


Figure1. Schematic description of an STM-Molecule-Silicon system partitioned into three parts, STM, substrate and device. The device levels are described by a suitable Hamiltonian  $H_D$ , the self-consistent potential  $U$  included the effect of electron-electron interaction under bias, and the contacts are described by energy-dependent self-energy matrices,  $\Sigma_1$  and  $\Sigma_2$ , that provide appropriate quantum boundary conditions. These elements are incorporated into an electronic structure calculation self-consistently combined with a non-equilibrium Green's function (NEGF) based quantum transport model.