

## **ABSTRACT**

### **Electron transport in gold chains: application and testing of the principal layer method**

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Recently, the theoretical description of electron transport in molecular wires has found much interest as a consequence of the experimental progress made in the field, in particular the scanning tunneling microscope (STM) and the mechanically controllable break junction (MCBJ). Here, a non-equilibrium Green's function formalism is used to describe the electron transport. The system is divided in three parts, the left and right electrodes and the wire. The electrodes do not interact directly, which is assured by means of a localized basis. The current through the molecule can be expressed in terms of its Green function where the effect of the electrodes is incorporated through their self energies.

In an initial study we investigate the distance dependence of the conductance between vacuum connected gold electrodes. Since we know that the conductance should decay exponentially with distance our study serves as a test for the applicability of the principal layer method. We find that an unphysical band can occur depending on the principal layer as well as on the buffer size. This unphysical band can be spotted in the band structure by its particular wide character. The contribution of this band to the conductance does not decay exponentially in contrast to the second band at Fermi level which contributes to the conductance as expected.

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