



KTH Theoretical Chemistry

# First principles simulations of electron transport at the molecule-solid interface

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# Abstract

In this thesis I concentrate on the description of electron transport properties of microscopic objects, including molecular junctions and nano junctions, in particular, inelastic electron tunneling in surface-adsorbate systems are examined with more contemplations. Boosted by the rapid advance in experimental techniques at the microscopic scale, various electric experiments and measurements sprung up in the last decade. Electric devices, such as transistors, switches, wires, etc. are expected to be integrated into circuit and performing like traditional semiconductor integrated circuit (IC). On the other hand, detailed information about transport properties also provides new physical observable quantities to characterize the systems. For molecular electronics, which is in the state of growing up, its further applications demands more thorough understanding of the underlying mechanism, for instance, the effects of molecular configuration and conformation, inter- or intra-molecular interactions, molecular-substrate interactions, and so on. Inelastic electron tunneling spectroscopy (IETS), which reflects vibration features of the system, is also a finger print property, and can thus be employed to afford the responsibility of single molecular identification with the help of other experimental techniques and theoretical simulations.

There are two parts of work presented in this thesis, the first one is devoted to the calculation of electron transport properties of molecular or nano junctions: we have designed a negative differential resistance (NDR) device based on graphene nanoribbons (GNRs), where the latter is a star material in scientific committee since its birth; The transport properties of DNA base-pair junctions are also examined by theoretical calculation, relevant experimental results on DNA sequencing have been explained and detailed issues are suggested. The second part focused on the simulation of scanning tunneling microscope mediated IETS (STM-IETS). We have implemented a numerical scheme to calculate the inelastic tunneling intensity based on Tersoff-Hamann approximation and finite difference method, benchmark results agree well with experimental and previous theoretical ones; Two applications of single molecular chemical identification are also presented following benchmarking.