Huckel I-V 3.0: A Self-consistent Model for Molecular Transport and its Applications

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Huckel I-V 3.0 is our latest transport model along the line of other Extended Huckel Theory (EHT) based models that we have developed earlier. In this model Non-equilibrium Green's Function (NEGF) formalism is coupled with EHT in order to describe transport through molecular systems. Significant improvements and modifications have been made in the description of the self-consistent potential. The Poisson part of the self-consistent potential is approximated by using CNDO (Complete Neglect of Differential Overlap) method which helps to simplify our procedure by avoiding the direct calculations of the time-consuming two electron integrals. The Laplace part of the self-consistent potential, as well as, the image potential (effect of the metallic electrodes surrounding the molecular device) is calculated using Finite Element Method (FEM) in 3D space. The self-consistent potential in Huckel I-V 3.0 incorporates both the charging and screening effects inside the molecule under applied bias and it retains the spatial features of the potential profile. As this model is based on semi-empirical methods it is computationally inexpensive compare to other ab-initio models yet at the same time it is able to preserve the complete accuracy in terms of physical characteristics.

We believe that Huckel I-V 3.0 can be a very useful model in explaining many different physical characteristics of molecular conductors that have been experimentally observed. We apply this model to investigate the origin of asymmetry in the current-voltage (I-V) characteristics observed in a recent break junction measurement for a symmetric molecule. We achieve good agreement between theoretical and experimental I-V characteristics, both in shape as well as overall magnitude. We conclude that such asymmetry arises due to unequal coupling with the contacts which generates asymmetry in charging. We also study alkanethiol I-V characteristics observed in a recent nanopore experiment. We achieve an excellent match between calculated and experimental results. One of the main features of Huckel I-V 3.0 is that a third terminal (as a gate) can be added to the system with relative ease. In order to showcase this strength of our model we perform three terminal calculations on single molecules. We study both alkanethiol chains and conjugated molecules as a molecular transistor and observe that alkanethiol molecules show better transistor performance.

A full journal publication of this work will be published in the Journal of Computational Electronics.

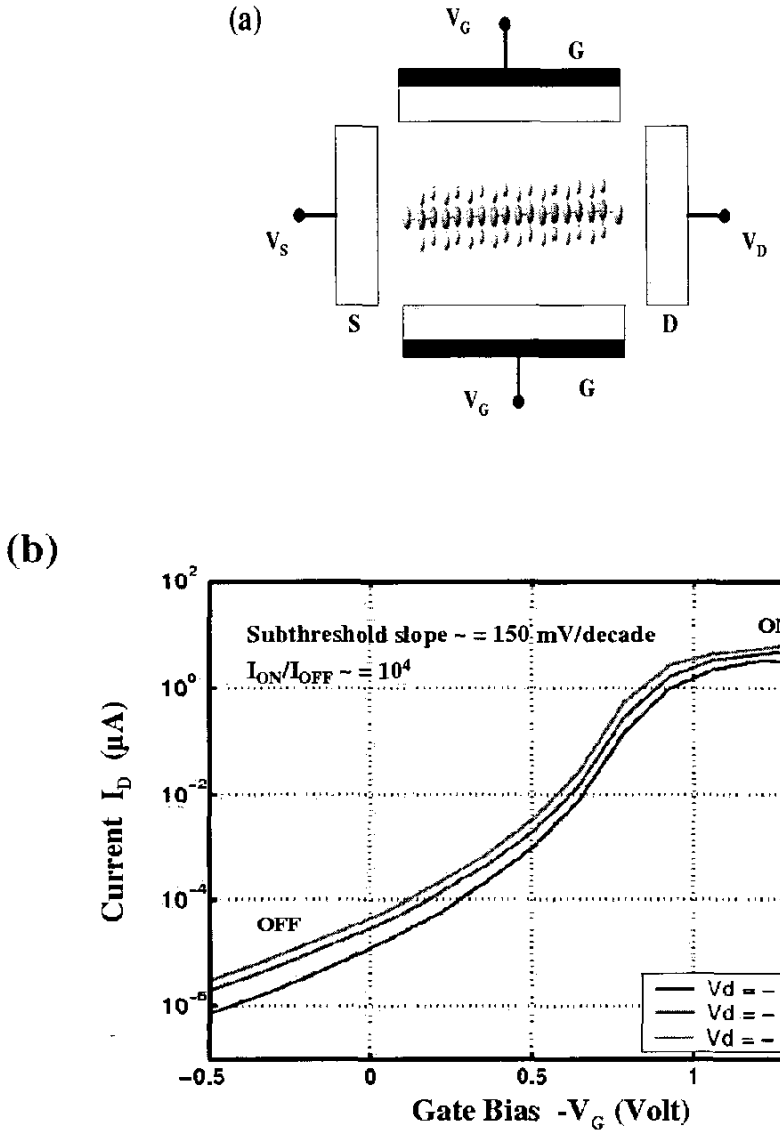

Figure 1: (a) a molecular transistor: HS-$(CH_2)_{16}$-SH molecule sandwiched between two gold contacts (treated as source and drain) and surrounded by four gate electrodes (two shown in the figure and the other two are out of the plane). The gate electrodes are placed 2 A° away from the molecule and the space in between is filled with SiO_2; (b) I_D-V_G curves for the above system. Alkanethiol molecules show better transistor performance (lower subthreshold slope and higher on-off current ratio) compare to that of conjugated molecules though the overall performance still remains below MOSFET devices.

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