Effect of charge transport in organic semiconductors on the conductance of silicon nanowires

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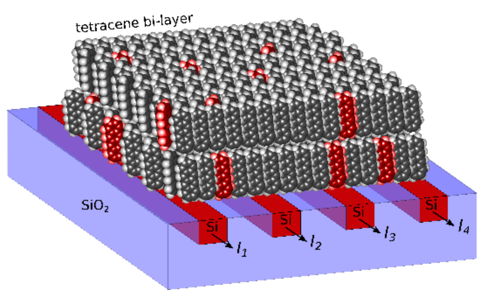
We study electron transport processes in a silicon nanowire covered by an organic semiconductor (see Fig. 1 a) [1]. We propose a mathematical model that estimates the effect of charge carriers in organic semiconductor (tetracene in this work) on the conductance of the nanowire. The model is based on the non-equilibrium Green's function approach [2] with the semi-empirical $sp^3d^5s^*$ tight-binding model for the electronic structure of the nanowire [3]. The scattering potential has been computed using a combination of the polarizable continuum model and density functional theory with the range-separated exchange-correlation functional for organic molecules [4].
Moving charge carriers in the organic semiconductor distort the electrostatic environment of the nanowire, introducing an additional source of elastic scatterings that suppresses the coherent transport of electrons. The computed conductance change caused by scattering on a single molecule is shown in Fig. 1b both for positive and negative charge carriers for a range of Fermi energies. There is also a possibility to observe the exciton and charge transfer across the interface between silicon and tetracene. In this case the organic semiconductor acts as a source of electrons and/or holes. A steady-state injection of additional charge carriers into the nanowire redefines the quasi-equilibrium thermodynamic variables such as temperature and Fermi energy level. In Fig. 1 b we have schematically shown the corresponding shift of the Fermi level, E_f, caused by the electron injection. As a result of such shift the conductance of the nanowire increases. Thus, in the considered case the movement of charge carriers in tetracene reduces the conductance of the nanowire introducing an additional source of scatterings, while the charge transfer across the interface enhances it. Both effects can be quantified from experimental measurement of the conductance.



a) b)

Fig. 1. a) an array of silicon nanowires covered by a bilayer of crystalline tetracene and b) conductance change in a silicon nanowire caused by scatterings on a single charge carrier.

References

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