Quantum and Spin Transport in Photoswitching Molecules

Anna Delin

Royal Institute of Technology

In recent years, functionality based on the spin of the electron has become ever more important in the electronics industry. The most famous application is probably the read-out devices based on the giant magneto-resistive effect. Many researchers and developers are looking for ways to cheaply mass produce identical devices on the scale of a few nanometers. One possible route is to make use of organic molecules, which tend to be stable, easy to synthesize in large quantities, and relatively simple to tailor according to what properties one is looking for. In this work, we investigate the finite-bias conduction properties of the photoswitching dithienylethene molecule attached to various electrode materials (Au, Ag, nonmagnetic Ni and spin-polarized Ni). The I-V characteristics are calculated using a non-equilibrium Green function technique and we discuss the role of molecule polarization and its effect on the conduction properties at finite bias. In particular, for the spin-polarized Ni electrodes, the I-V characteristics for the spin up and spin down channels are found to be very similar, despite the fact that the Ni electrode density of states is very different for spin up and spin down (Ni is known to be a so-called strong ferromagnet meaning that it is almost completely spin polarized at the Fermi level). This implies that the number of d-states at the Fermi level appear to play a minor role for the conduction of the Ni-dithienylethene-Ni system. This conclusion also agrees well with what we find when comparing Ag and Au electrodes with nonmagnetic Ni electrodes.