Photoinduced control of single molecule conductance

Ya.R. Zelinskyy and E.G. Petrov

Bogolyubov Institute for Theoretical Physics, National Academy of Science of Ukraine, 14-B Metrologichna Str., 03680 Kiev, Ukraine, E–mail: yzelinskyy@bitp.kiev.ua

Due to a potential application of single molecules as basic elements for a future electronics, the studies of conductive properties of organic molecules have attracted considerable interest. Molecular devices (single molecules embedded in between two metallic electrodes) are already fabricated with different functional properties like as a current rectification and a switching effect. Special interest has been focused on the role of external time-dependent fields controlling the conductance of single molecules. In particular, the use of electromagnetic radiation such as a laser light, can provide a convenient method to operate a single-molecule conductance.

To gain insight into investigation of a photoinduced single-molecule conductance, we propose a model where the photoinduced current is formed through a specific type of molecule (connecting two nanoelectrodes) which exists in its neutral, single-charged and photoexcited states. In this model, the conductance is governed by a specific charge-transfer processes. Respective kinetic equations are derived with use of nonequilibrium density matrix method. Exact solution of the closed set of kinetic equations is applied to analyze a time-dependent current formation. For a steady state regime, the analytical expression for a combine elastic and inelastic photoinduced inter-electrode current is derived. The influence of light frequency on current-voltage and conductance-voltage characteristics is analyzed in detail. The effect of photoinduced switching between the low and the high molecular conductance states is theoretically predicted. Additionally, in the case of asymmetric voltage drop across the molecule, a current rectification is observed.