

Field-induced inversion of resonant tunneling currents through single molecule junctions and the directional photo-electric effect

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It has been known for several decades that the electric current through tunneling junctions is affected by irradiation of the external leads. In particular, photon-assisted currents were demonstrated and studied extensively in tunneling junctions of different compositions, and for different radiation wavelengths. In this work this phenomenon is revisited in the context of single molecule junctions. Restricting the theoretical discussion to adiabatic periodic driving of the leads within a non-interacting electron formulation, the main features of specific molecules are encoded in the discrete electronic energy levels. The detailed level structure of the molecule is shown to yield new effects in the presence of asymmetric driving. In particular, when the field-free tunneling process is dominated by a single electronic level, the electric current can flow against the direction of an applied static bias. In the presence of a second electronic level, a directional photo-electric effect is predicted, where not only the magnitude but also the direction of the steady state electric current through the tunneling junction can be changed by a monotonous increase of the field intensity. These effects are analyzed and explained by outlining the relevant theory, using analytic expressions in the wide-band limit, as well as numerical simulations beyond this limit.