

Abstract Submitted
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Optical properties of current carrying molecular wires MICHAEL GALPERIN, Northwestern University, ABRAHAM NITZAN, Tel Aviv University — We consider several fundamental optical phenomena involving single molecules in biased metal-molecule-metal junctions. The molecule is represented by its highest occupied and lowest unoccupied orbitals, and the analysis involves simultaneous consideration of three coupled fluxes: the electronic current through the molecule, energy flow between the molecule and electron-hole excitations in the leads, and the incident and/or emitted photon flux. Using a unified theoretical approach based on the non-equilibrium Green function method we derive expressions for an absorption lineshape (not an observable but a useful reference for considering yields of other optical processes) and for the current induced molecular emission in such junctions. We find that current driven molecular emission and resonant light induced electronic currents in single molecule junctions can be of observable magnitude under appropriate realizable conditions. In particular, light induced current should be observed in junctions involving molecular bridges that are characterized by strong charge transfer optical transitions. For observing current induced molecular emission we find that in addition to the familiar need to control the damping of molecular excitations into the metal substrate the phenomenon is also sensitive to the way in which the potential bias is distributed on the junction.

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