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Theory of electron-vibration coupling in the electron transport of molecular bridges MASARU TSUKADA, Waseda University, KUNIHIRO MITSUTAKE, Canon Research Center, Canon Inc. — Electron transport through molecules connecting nano-electrodes is the key issue for molecular devices. The competition and coexistence of the coherent and dissipative transport are unresolved issue, in spite of its importance. In this work, this problem is investigated by a novel theoretical approach of an *ab initio* molecular orbital model with combining polaron effect. When carriers are injected into molecules from electrodes, the structure of the molecule changes, which leads the coupling term of the electron/hole and the molecular vibration. The model Hamiltonian for the thiophene oligomer is solved by a variational approach, and a mixed states of dressed polaron with molecular orbital states mediated by the phonon cloud is found. The former and latter are predominant for small or large transfer integral, respectively. The excited states can be calculated in the same framework as the ground state. The overall carrier transport properties can be analyzed by solving the master equation with the transition rate estimated by the golden rule including the phonon degrees of freedom. In this theoretical approach, the coherent and dissipative electron transport through molecular bridges can be described in a uniform systematic way.

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