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Vibronic coupling effect on the electron transport through molecules MASARU TSUKADA, Waseda University, KUNIHIRO MITSUTAKE, Canon Research Center, Canon Inc. — Electron transport through molecular bridges or molecular layers connected to nano-electrodes is determined by the combination of coherent and dissipative processes, controlled by the electron-vibron coupling, transfer integrals between the molecular orbitals, applied electric field and temperature. We propose a novel theoretical approach, which combines *ab initio* molecular orbital method with analytical many-boson model. As a case study, the long chain model of the thiophene oligomer is solved by a variation approach. Mixed states of moderately extended molecular orbital states mediated and localised by dress of vibron cloud are found as eigen-states. All the excited states accompanied by multiple quanta of vibration can be solved, and the overall carrier transport properties including the conductance, mobility, dissipation spectra are analyzed by solving the master equation with the transition rates estimated by the golden rule. We clarify obtained in a uniform systematic way, how the transport mode changes from a dominantly coherent transport to the dissipative hopping transport.

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