

Abstract Submitted
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Detection of Inelastic Electron Transport Properties in Molecular Junctions by Internal Substitutions HISAO NAKAMURA, Department of Chemical System Engineering, the University of Tokyo — Doping and chemical substitutions for molecules is one of promising technique to control the $I - V$ characteristic and engineering of molecular devices. In this presentation, we propose an idea of *internal* substations to detect ballistic and inelastic transport in molecular junctions. We adopt the benzene-dithiol as a template molecule and apply first principle transport calculations, which are based on nonequilibrium Green's function combined with density functional theory, to several internally substituted systems. The inelastic transport is treated within the conventional lowest order expansion (c-LOE) formalism. By comparison of substituted systems, we show systematic analyses of electron tunneling pathway for both ballistic and inelastic currents as well as electron-phonon couplings on bridge molecules. The correlation of inelastic electron tunneling spectroscopy (IETS) and Raman spectroscopy will be also discussed.

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