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Electron Transport and Thermoelectricity in Alkanethiol Molecular Junctions[1] YU-CHANG CHEN, CHUN-LAN MA, DIU NGHIEM, YU-SHEN LIU, Department of Electrophysics, National Chiao Tung University, Taiwan — We investigate the electron transport properties of alkanethiol molecules in the two- and three-terminal junctions by using first-principles approaches. We observe that novel states around the Fermi levels are introduced in the amino-substituted butanethiol junction. It leads to a sharp increase of the current owing to the resonant tunneling. We also describe a field-theoretic theory combined with first principles approaches to calculate the thermoelectricity. The dependence of the Seebeck coefficient on the biases, gate voltages, and temperatures is systematically investigated. Due to the novel states introduced by the amino-substituted butanethiol junction, the Seebeck coefficient could be easily controlled by using gate voltages and biases. When the temperature in one of the electrodes is set to zero, the Seebeck coefficient could vary pronouncedly with the temperature in the other electrode, and such dependence could be enhanced by varying gate voltages. At finite biases, we also find richer features in the Seebeck coefficient related to the density of states in the vicinity of the left and right Fermi levels.

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