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### First Principles Study of the Electron Transport Properties of Buthane-dithiol Nano-Molecular Wire

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#### Abstract:

We report a first-principles study of electrical transport in a single molecular conductor consisting of a buthane-dithiol sandwiched between two Au (100) electrodes. We show that the current was increased by increasing of the external voltage biases. The projected density of states (PDOS) and transmission coefficients (T(E)) under various external voltage biases are analyzed, and it suggests that the variation of the coupling between the molecule and the electrodes with external bias leads to the increase of the current. Therefore, we propose that the most origin of electron transport mechanism in molecular devices is caused by the characteristics of both the molecule and the electrodes as well as their cooperation, not necessarily only by the inherent properties of certain species of molecules themselves.

**Keywords:** single molecular conductor, Au(100) electrodes, DFT, buthane-dithiol

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