# INELASTIC TRANSPORT THEORY FOR NANOSCALE SYSTEMS: LOCAL HEATING IN A Cu–$C_{60}$–Cu JUNCTION

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When an electric current is passed through a nanoscale device – such as a single molecule or an atomic-size contact – the junction will heat up due to excitation of nuclear vibrations. In this presentation we describe results using a first-principles computational scheme for calculating conductance properties of nanoscale systems, taking into account inelastic scattering and energy dissipation [1]. The methods are based on a combination of density functional theory (DFT) and nonequilibrium Green's functions (NEGF) [1,2]. It involves quantitative calculations of electronic structure, vibrational modes and frequencies, electron-phonon (e-ph) couplings, and inelastic current-voltage characteristics in the weak e-ph coupling limit.

Specifically we consider the transport through individual $C_{60}$ molecules on a Cu(100) surface contacted with the tip of a scanning tunneling microscope (STM) [3]. As a model for the system we work with the supercell structure shown in Fig. 1. Depending on the tip-molecule distance we find that the conductance varies several orders of magnitude. In the tunneling regime the conductance varies exponentially with distance. In the contact regime, when the tip comes sufficiently close – and a bond is formed between the tip apex and the $C_{60}$ molecule – the conductance levels off to reach a plateau. In the transition region between these different regimes our calculations show how the conductance is affected by current-induced fluctuations that modulate the tip-molecule distance. From an analysis of the vibrational excitations we quantify the local heating and extract the bias-dependent effective temperature of the junction.

**References:**

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**Figures:**

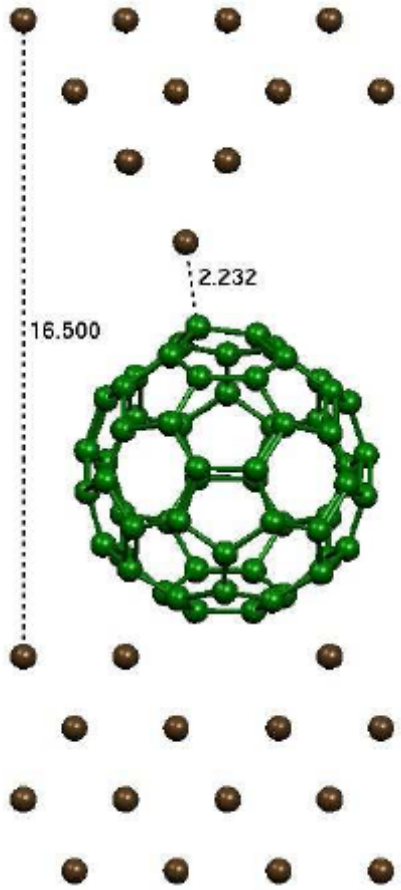


**Fig. 1:** Side view of the $C_{60}$-Cu(100) supercell used in the transport calculations.