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Ab initio study of inleastic transport in molecular electronic devices NIKOLAI SERGUEEV, University of Texas at Austin, ALEX DEMKOV, University of Texas at Austin — One of the most important issues of conduction at nano-scale concerns the effects of atomic vibration. Interaction between electrons and vibrational excitations in nanoelectronic devices has become the problem to solve in order to advance the research field of nanoelectronic theory. Understanding these effects is crucial for predicting device performance. In this talk, we present a method based on Density Functional Theory and Nonequilibrium Green's functions formalism for the calculation of tunneling current and conductance in molecular electronic devices in the presence of electron-phonon interaction. Using self-consistent Born approximation, we can determine the phonon self-energy, the electron Green's function, the electronic density matrix and the electronic Hamiltonian within equal footing of our formalism. As an example, we present numerical results obtained for several molecular electronic devices and show that only few molecular vibrational excitations seem to have an effect on the inelastic tunneling.

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