

Ballistic Transport in Nanostructures, and its Application to Functionalized Nanotubes

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Abstract— We developed and implemented a first-principles based theory of the Landauer ballistic conductance, to determine the transport properties of nanostructures and molecular-electronics devices. Our approach starts from a quantum-mechanical description of the electronic structure of the system under consideration, performed at the density-functional theory level and using finite-temperature molecular dynamics simulations to obtain an ensemble of the most likely microscopic configurations. The extended Bloch states are then converted into maximally-localized Wannier functions to allow us to construct the Green's function of the conductor, from which we obtain the density of states (confirming the reliability of our microscopic calculations) and the Landauer conductance. A first application is presented to the case of pristine and functionalized carbon nanotubes.

[Full Text Not Available]