Applications of First Principles Simulations of Quantum Transport

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I will describe the TranSIESTA method to describe the electronic transport properties of nanoscale devices out of equilibrium. The method is based on a Non-Equilibrium Green's Function formulation of the transport problem, together with a Density Functional Theory description of the electronic potential. I will briefly discuss the basic features of the method, and also its limitations and shortcomings, and then I will mainly present examples of different applications in the context of Scanning Tunneling Spectroscopy (STS), molecular bridges, and solid state ferroelectric tunneling junctions.

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