TranSIESTA: Advanced Applications in Electrochemistry and Spintronics

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SIESTA [1,2] is a Density Functional Theory (DFT) code that uses localized, numerical atomic orbitals as a basis set, and is designed to be able to deal with systems with very large numbers of atoms. One of the distinctive features of SIESTA compared with other DFT codes is the possibility to deal with open systems connected to semi-infinite electrodes at different electrochemical potentials. This non-equilibrium situation is handled through the use of the Non-Equilibrium Green's Functions (NEGF) formalism combined with DFT [3]. This is implemented in the TranSIESTA module of SIESTA, and was originally developed to describe electronic transport in nanoscale devices in molecular electronics and nanoelectronics, where quantum effects (ballistic transport, tunneling, conductance quantization, quantum confinement, etc) are of paramount importance [4]. TranSIESTA was continuously improved, with more efficient numerical algorithms and capabilities, like the possibility of including bias voltages through gates, and multiterminal setups [5].

Recent work has recently enhanced the applicability of TranSIESTA to problems beyond electronic transport. Two of these will be the topic of this talk. The first one is the study of electrochemical processes, where an electrolyte is in contact with metallic electrodes which are subject to external voltages. These problems are formally very similar to those involving electronic transport in nanoelectronic devices (as the electrodes are subject to different electrochemical potentials) although in this case the electrical current is due to the ionic dynamics at the electrolyte and the chemical reactions at the electrolyte-electrode interface. The second topic is that of spintronics, involving spin polarized currents. TranSIESTA has been revamped to be able to treat with such problems, not only including spin polarization, but also the description of non-collinear spin states (where the direction of magnetization can change in space, like in the case of ferromagnetic domain walls), and spin-orbit effects, which are key for spintronic applications.

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