Matlab Implementation of Extended Hückel Tight Binding Methods and its Application in Spin Transport Calculations

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Ohm's law works very well for macroscopic systems. It provides a quick and easy way to evaluate transport properties at the macroscopic scale. However, when the system scale becomes smaller, Ohm's law does not apply anymore. It is over-simplified to precisely describe the electron transport properties at the mesoscopic as well as the atomistic scale.

To describe transport in magnetic devices such as sensors and memories and to achieve fast progress in newly proposed material systems, a very accurate description of the transport on the atomistic level with the flexibility to describe structural complicated systems is needed. Density functional theory can provide accurate information of many material systems but is usually numerically very challenging for complicated structures. The Extended Hückel Tight Binding Methods (ETH-TB) in combination with density functional theory can provide a model based on a few physical parameters with the accuracy of density functional theory. The MATLAB Optimization toolbox allows to perform a multi-dimensional fitting algorithm to obtain the ETH-TB parameters from first principle band structure models. To speed up this process we have also implemented a version in which relevant processes can be run in parallel. Within the obtained non orthogonal Extended Hückel Tight Binding scheme we have developed a multiband transport code. We demonstrate how we construct the Hamiltonian as well as the Overlap matrix and how we calculate the transmission properties of the given system using the Green's functional formalism.