MATDCAL: a first principles package for nanoelectronics modeling

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Abstract

We report an ab initio software package MATDCAL for investigating electronic transport properties in nano electronic devices. MATDCAL is based on carrying out real space density functional theory (DFT) within the Keldysh nonequilibrium Green function (NEGF) framework. The code is mainly written in MATLAB, combining with numerically intensive part in Java for efficiency. In order to realize parallelization in MATLAB, we have implemented a C-interface in MATLAB to link to MPI. MATDCAL is the first MATLAB-based electronic package for nanoelectronics research that is based on atomistic first principles. We report some implementation issues using MATLAB for large scale physics computation. Several examples will be given on quantum transport analysis of nano-scale devices.