Multiple electrode (Ne1) support in the DFT+NEGF code TranSIESTA

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Publication date:
2015

Document Version
Publisher's PDF, also known as Version of record

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Citation (APA):
Multiple electrode \((N_e \geq 1)\) support in the DFT+NEGF code TranSIESTA

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# Introduction

Density functional theory based non-equilibrium Green function methods (DFT+NEGF) are by now standard for calculation of transport properties in nanostuctures. In the TranSIESTA code [1, 2] the NEGF implementation is currently scaling with \(N^2\) which limits the number of orbitals used, \(N\) being number of orbitals. In this work we present a re-implementation of TranSIESTA which scales linearly in system size (order-\(N\)) and allowing for multiple electrodes \((N_e \geq 1)\) in a flexible manner [3]. In conjunction with TranSIESTA we report on an optimised \(t\)b\(r\)\(a\)\(n\) code which enables, 1) \(N_e \geq 1\) electrodes, 2) interpolation of Hamiltonian between bias, 3) projection of molecular Hamiltonians, 4) custom tight binding and 5) phonon transport.

# Efficiency of improved TranSIESTA DFT-NEGF method

The non-equilibrium Green function equations

\[
\rho_{nm} = \frac{1}{\pi} \int \frac{d \omega}{d k} \left( \frac{1}{\omega - \epsilon_m - G_{nn}^{\uparrow} + i \eta} - \frac{1}{\omega - \epsilon_n - G_{nn}^{\downarrow} + i \eta} \right) \delta(\epsilon_m - \epsilon_n)
\]

- **Different inversion algorithms**, 1) Block-tri-diagonal (BTD), 2) MUMPS, 3) LAPACK
- **Efficient pivoting to obtain good scalability on BTD inversion
- **Example of possible geometries**

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**Example — NEGF calculation of graphene T-junction**

- NEGF calculation of 3 (left-right-top) electrode, periodic in the arm-chir direction.
- Compared against pristine graphene transmission spectrum
- Spectral density, GF(G) of states on atom closest to basal graphene plane in T-junction

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**Example — Molecular projection transmission**

- Full spectroscopic analysis using linear (Löwdin) projected Hamiltonians to attribute transport to molecular levels
- Graphene phonon transport along zig-zag direction
- Bulk Silicon phonon transport along 100 direction
- Reads GULP [4] output to create Hessian (dynamical) matrix, easily extendable to other

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**Conclusion**

- **Full \(N_e \geq 1\) NEGF calculations in TranSIESTA**
- **Huge performance improvement for higher throughput and larger systems
- **Huge memory reduction due to implemented sparse algorithms
- **Versatile transport calculator \(t\)\(b\)\(r\)\(a\)\(n\)\(t\)rans
  - Interpolating bias calculations
  - Molecular projected transmission spectrum
  - Implict tight-binding calculations using simple scripting language (Python)
  - Bond-currents for orthogonal basis sets

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Release in late 2015

Speak with

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