WORKSHOP

25 - 27
October 2017

Seminar Room,
Danchip - DTU,
Denmark

Workshop
coordinated by
Nick R. Papior and
DTU Nanotech

REGISTER
to participate

>>Multi-electrode nanoscale transport with non-equilibrium Greens functions: From tight-binding to DFT<<

DTU Nanotech and Center for Nanostructured Graphene proudly invites you to the second TranSIESTA and TBtrans workshop with hands-on focus on the software.

This workshop is a 3-day course aimed at researchers interested in performing large-scale tight-binding transport calculations and/or density-functional theory + non-equilibrium Green function transport calculations. The workshop is free to attend with lunches included.

The tutorial is an initiative of the DTU Nanotech and Center for Nanostructured Graphene.

It is mandatory that you REGISTER HERE to participate in this free workshop.

Accommodation is at the expense of the participants.

ABSTRACT *for*

>> Multi-electrode nanoscale transport with non-equilibrium Greens functions: From tight-binding to DFT<<

Seminar Room,
Danchip - DTU,
Denmark

Link to
Accomodation

Travelplan
from Copenhagen

This 3-day workshop concentrates on the TBtrans/TranSiesta implementation of the nonequilibrium Green function techniques. The focus will be tutorials and hands-on experience with the transport utility TBtrans and the self-consistent method TranSiesta.

Our workshop will start by introducing the Green function method to a required level of understanding for the remainder of the workshop. Tutorials starts with simple tightbinding models created by Python scripts using Sisl. The input options for TBtrans will be explored and details regarding the TBtrans utility will be emphasised. Simultaneously, data-analysis will be presented using Python. Succeeding the TBtrans tutorials we will concentrate on self-consistent non-equilibrium calculations using TranSiesta. We will showcase how to perform N electrode calculations using TranSiesta.

Upon completing the tutorial the attendee should have obtained knowledge on how to conduct tight-binding calculations as well as self-consistent non-equilibrium Green function calculations.

Prerequisites *for*

>> Multi-electrode nanoscale transport with non-equilibrium Greens functions: From tight-binding to DFT<<

- The participants are required to have a basic knowledge of solid state physics.

- The participant should bring a laptop with a Linux/MacOS installation. You are free to use Virtual Box if you are more comfortable with Windows.

- The participants are required a basic knowledge of command-line use (See e.g. this site: http://linuxcommand.org/learning_the_shell.php).

- The participants should, preferentially, have a basic knowledge of Siesta and be able to conduct Siesta calculations.

- The participants should, preferentially, have a basic knowledge of Python coding and in particular the NumPy package.

Registration is Mandatory to participate in this free workshop!!

REGISTER HERE
to participate

DTU

DTU Nanotech
Department of Micro- and Nanotechnology

Center for Nanostructured Graphene

VILLUM FONDEN

Program *for*

>> Multi-electrode nanoscale transport with non-equilibrium Greens functions: From tight-binding to DFT<<

The program of the tutorial is currently comprising the following:

25 October	08:30-09:00	*Registration*
	09:00-10:00	**Theory 1: Non-equilibrium Green function therory**
	10:00-10:30	*Break*
	10:30-12:00	**Theory 2: Non-equilibrium Green function therory**
	12:00-13:00	*Lunch*
	13:00-15:00	**Tutorial 1: Tight-binding and TBtrans**
	15:00-15:30	*Break*
	15:30-17:00	**Tutorial 2: Tight-binding and TBtrans**
26 October	08:30-09:00	*Registration*
	09:00-10:00	**Tutorial 3: Advanced tight-binding for TBtrans (N-electrode)**
	10:00-10:30	*Break*
	10:30-12:00	**Theory 3: Introduction to TranSiesta**
	12:00-13:00	*Lunch*
	13:00-15:00	**Tutorial 4: TranSiesta calculations (part 1)**
	15:00-15:30	*Break*
	15:30-17:00	**Tutorial 5: TranSiesta calculations (part 2)**
27 October	08:30-09:00	*Registration*
	09:00-10:00	**Theory 4: NEGF for N-electrode calculations**
	10:00-10:30	*Break*
	10:30-12:00	**Tutorial 6: TranSiesta calculations for N-electrodes**
	12:00-13:00	*Lunch*
	13:00-15:00	**Tutorial 7: Continuing TranSiesta calculations for N-electrode**
	15:00-15:30	*Break*
	15:30-17:00	**Wrap-up: Recap important points of calculation setups**