OPEN KNOWLEDGE PROGRAM

MODULE 7 - *TBtrans* AND *TranSiesta* TUTORIAL: NON-EQUILIBRIUM GREEN FUNCTIONS, FROM TIGHT-BINDING TO SELF-CONSISTENCY

9, 10 AND 11 NOVEMBER 2016

9, 10 and 11 November 2016

ICN2 Seminar Hall, ICN2 Building, UAB

Module coordinated by **Nick R. Papior** and **HR & Education Dept.**

ICN2 proudly invites you to the seventh ICN2 Open Knowledge (OK) Program edition. As in previous OK Program editions, these series of talks offer a high scientific level and a global overview of the matter suitable for all kinds of researchers and advanced physics students.

Please note that the format of this edition is different. It consists of three consecutive days of theoretic and practical sessions. For participants to have the most satisfactory experience some prerequisites should be met and you should bring your own laptop (see prerequisites below).

The ***TBtrans*** and ***TranSiesta*** tutorial is an initiative of the ICN2 *Theory and Simulation* Group, in the context of the projects **MaX** and **NFFA**.

It is mandatory that you **REGISTER HERE** to participate in this free workshop. **The deadline to register is Friday 28th of October, 2016.**

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Abstract

This 3-day workshop concentrates on the ***TBtrans/TranSiesta*** implementation of the non-equilibrium 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.

Location
Seminar Room, ICN2 Building
UAB Campus, Bellaterra (Barcelona), 08193, Spain

Close accommodation can be found at
Hotel Campus UAB, Barcelona which is located on campus and a 10 minutes walk from ICN2.

DOWNLOAD HERE the registration form to stay at the UAB Campus Hotel (www.hotelcampusuab.com).

For transportation you may locate ICN2 using the instructions found here: http://icn2.cat/en/contact

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Prerequisites

- 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.

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Program

The program of the tutorial is currently comprising the following:

9 November

08:30 - 09:00	Registration
09:00 - 10:00	**Theory 1:** Non-equilibrium Green function theory
10:30 - 12:00	**Theory 2:** Non-equilibrium Green function theory
12:00 - 13:00	Lunch
13:00 - 15:00	**Tutorial 1:** Tight-binding and TBtrans
15:30 - 17:00	**Tutorial 2:** Data analysis for TBtrans

10 November

09:00 - 10:30	**Tutorial 3:** Advanced tight-binding for TBtrans (N-electrode)
11:00 - 12:00	**Theory 3:** Introduction to TranSiesta
12:00 - 13:00	Lunch
13:00 - 15:00	**Tutorial 4:** TranSiesta calculations (part 1)
15:30 - 17:00	**Tutorial 5:** TranSiesta calculations (part 2)

11 November

09:00 - 10:30	**Theory 4:** NEGF for N-electrode calculations
11:00 - 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
15:30 - 17:00	**Wrap-up:** Recap important points of calculation setups