

# 1 CECAM Tutorial & Workshop

”High performance models for charge transport in large scale materials systems”

October 5<sup>th</sup> - 10<sup>th</sup> 2014

Bremen Center for Computational Materials Science

University of Bremen

Supported by:

cecam-MM1P.de

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University of Bremen

Organised by:

Tim Wehling (University of Bremen)

Aldo di Carlo (University Tor Vergata Rome)

Thomas Frauenheim (University of Bremen)

Homepage:

<http://www.cecam.org/workshop-1033.html>

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## 1.1 CECAM Workshop Scientific Report

- Workshop: "High performance models for charge transport in large scale materials systems"
- Organizers:
  - Tim Wehling (University of Bremen)
  - Aldo di Carlo (University Tor Vergata Rome)
  - Thomas Frauenheim (University of Bremen)
- Location:
  - University of Bremen, Germany,
  - October 4<sup>th</sup> until October 10<sup>th</sup>

### *I Summary*

The rise of novel materials for energy harvesting, energy storage and optoelectronic applications and the rush for device miniaturization, driven by the needs of computer industry, pose new challenges in modeling the physics of charge transport. Industry is moving massively towards novel materials: polymer and organic materials nowadays are routinely employed. Organic and inorganic 1D and 2D materials are gathering large attention, single molecule devices could play a role in the emerging field of spintronics. The landscape of novel materials is that rich that high-throughput Computer Aided Design (CAD) techniques are foreseen for the near future. Even in traditional electronic devices, the design of silicon-based transistor has been moved to multi-gate structures to keep up with Moores scaling law, and the boundary between device and materials design is becoming more and more evanescent.

The primary objective of the proposed workshop is to interconnect different communities involved in charge transport modelling working on large scale atomistic simulations of materials and devices, regardless the specific technological subarea of interest. The workshop will focus on computational and theoretical challenges and techniques, to encourage a strong multidisciplinary approach. We aim for encouraging dialogue between ab-initio, semi-empirical and empirical methods communities. In order to foster such an exchange internationally leading groups in multiscale physics approaches and coupling will be invited. Given the strongly interdisciplinary scope of the workshop, only theoretical modelling groups will be invited in order to ensure a sharp focus on theoretical method developments for next generation high performance models for charge transport in large scale materials systems. About 30 leading experts in the fields of ab initio methods and techniques

- Density-functional based tight binding - DFTB
- Empirical tight-binding - ETB
- Coarse grained fragment orbital methods

- Kernel polynomials and
- FEM-atomistic coupling

Have been invited, and gave keynotes on the related areas to set the stage and define the targets for future developments. The programme consisted of 32 invited talks of 40 minutes (35+5) each and one poster session presenting 44 posters. In addition, many social events (reception and conference dinner) to allow for informal exchange were held. The invited talks were given by well-established scientists from the different communities, both theoretical and experimental, which acted as platform for interesting cross-interdisciplinary discussions. The invited talks were followed by a poster session where the participants could show their scientific work and exchange of ideas with a broad knowledge in oxide chemistry/physics. The organization was very compact with the scientists accommodated in the same hotel fostering exchange and discussion between the participants also outside the meeting room.

Prior to the workshop, October 5th and 6th 30 young researchers participated in an Hands-on-Tutorial to become trained in advanced quantum transport simulations using the DFTB+ software. Furtheron Gerhard Klimeck (Purdue University) and Matthias auf der Maur (University Tor Vergata, Rome) introduced the participants into the simulations using the commercial software packages NANOHUB and TiberCad.

Financial support from the German CECAM node multi-scale modelling from first principles, cecam-mm1p.de, the University Bremen, Psik and the European Science Foundation is gratefully acknowledged.

## ***II Scientific content, main outcome of key presentations***

The workshop succeeded in the following objectives:

- 1) To share the state of the art at a computational level, regarding performance, scalability, parallelization and hence range of applicability of different charge transport techniques. To define common targets for method developments between different communities, focusing on hierarchical and domain multiscale coupling techniques, interconnection between electronic structure methods, KPM methods and to FEM-methods. Establishing the natural link between (semi)-ab initio DFTB and KPM methods to treat transport and electron dynamics efficiently in complex materials for next generation electronic applications.
- 2) To set up, share and investigate current and novel multiscale approaches combining atomistic description of the charge transfer process, classical force field dynamics, Monte Carlo and Finite Element description of the material, in order to develop methodologies towards the simulation of realistic structures, estimating and possibly including the effects of thermal fluctuations, configurational and statistical disorder.
- 3) To share the perspectives for the next years of research in the field, in particular referring to novel emerging issues such as time-dependent non equilibrium phenomena in complex systems.
- 4) To promote the creation of international collaboration networks in order to improve the interdisciplinary approach and connect scientists coming from physics, quantum chemistry, and electronic engineering communities.

### ***III Scientific advances expected for the next 4 years***

The talks and discussion during coffee breaks identified different key-advances in different areas.

*Note: 1) desktop computing, 2) departmental machines, 3) national supercomputers, 4) Current European Supercomputers (PRACE resources) 5) Leading edge peta-flop or exa-flop machines.*

#### **Electronic and excitonic transport in organic semiconductors (small molecules)**

Tremendous progress have been made in recent years concerning ab-initio calculation of Marcus transfer rates. In order to further advance the field for improving predictivity, we need to develop

(i) methods capable of assessing molecular morphologies and self-assembling properties of soluble organic semiconductors and interfaces. (2,3,4)

(ii) methods for quantitative description of electrostatic and polarization effects (0.1eV accuracy) in large-scale molecular morphologies using combined QM/MM/FEM methods (3,4)

(iii) cost-efficient methods for excited states, especially in a polarizable/electrostatic environment (3,4,5)

(iv) techniques for constructing diabatic (localized) states in large and partially ordered morphologies (3,4,5).

(v) charge/exciton transfer theories beyond semi-classical high-temperature limits.

#### **Hybrid interfaces and charge injection**

In order to improve and understand charge injection at the interfaces, we need to develop

(vi) reliable methods for predicting morphologies of organic compound at metallic or semiconducting interfaces. (3,4)

(vii) computation of electronic states of molecules near interfaces including polarizable environments (3,4,5)

(viii) computation of electronic states of molecules near interfaces including polarizable environments (3,4,5)

(ix) new methods to compute charge injection mechanisms at interfaces including hopping and partially coherent transport mechanisms such as tunneling (3,4)

#### **Charge transport in inorganic semiconductors (nanowires, nanotubes, 2D materials)**

Charge transport in inorganic nanostructures requires systematic calculations of electron-phonon interactions. Many problems in nanodevice transport are currently tackled with time-consuming non-equilibrium Greens functions approaches. In order to advance de field we need to develop

(i) Reliable calculations of materials morphologies, especially disordered interfaces (e.g., Si/SiO<sub>2</sub>). (3,4)

(ii) Reliable calculations of electron-phonon couplings and efficient calculations of transport including elastic and inelastic scattering. (3,4)

(iii) calculation of heat transport and heat dissipation, crucial for ultrascaled electronic nanodevices. (2,3,4)

(iv) combined QM/MM calculations to build realistic models for contacts and their electronic properties (e.g. Ti/MoS<sub>2</sub>, Pd/CNT, ). (2,3,4)

### *III. Assessment of the results and impact on future directions of the field EU2020*

The workshop identified three main aspects to be related to current and future funding opportunities:

1) The topic calls for highly interdisciplinary approaches, ranging from basic theoretical physics to electronic engineering. All these communities were represented by several speakers during the workshop.

2) A strong effort is devoted to efficient peta-scale numerical simulation schemes and most of the computational results shown can only be obtained on HPC systems.

3) The technology transfer process between academy, spinoff enterprises, small medium enterprises (SMEs) and large enterprises (LEs) is short, a fact proved by the participation of industrial representatives from US and Europe. All these points are well represented in the funding scope of the HORIZON2020 European Framework Program. Interdisciplinarity and involvement of SMEs calls especially for large collaborative projects. These concepts are relevant to the 2014-2015 HORIZON2020 calls (FETPROACT1, FETHPC1) both in the ICT and NMP funding programmes, and to two pillars (out of three) of the HORIZON2020 funding scheme: emphasis on excellent science and industrial innovation and leadership. The most relevant may include:

1) Multiscale modelling of organic electronic devices from ab-initio to mesoscopic and to device-scale simulations. This is not only relevant to academy, but to SMEs active in the industrial field of scientific modelling and SMEs and LEs developing materials and devices.

2) Advances in ab-initio and QM/MM simulations methods, typically developed for organic compounds, to be extended to inorganic materials and inorganic and hybrid interfaces.

### *IV Scientific importance for European Industries*

Progress in the field of charge transport in materials and devices is fundamental to many European industries connected to high-tech, material manufacturing and ICT. During the workshop several speakers reported on collaborations with key industries. Examples are

- ST Microelectronics for Si nanodevices, Si Nanowires.
- Thales for Graphene and carbon based materials
- Airbus for Conducting polymers and nanocomposites, metamaterials.
- BASF for development of novel organic materials.

- Infineon for novel electronic devices
- Philips for novel light emitting devices (LEDs, OLEDs)
- OSRAM for novel light emitting devices (LEDs, OLEDs)

Such collaborations can be strengthened by focused research projects for the development of new materials and devices in key enabling technologies. The field of nanodevices is currently opening to new materials, especially 2D. The EU flagship on graphene and 2D materials is indeed expected to produce several new outcomes. However, technological innovation is not limited to these novel materials. Organic compound for transparent electronics and organic light emitting devices or cheap photovoltaics are highly desirable and represent a very active field of research where challenging modeling problems have to be tackled in order to provide timely answers to industrial needs, reducing development times. Nanoscale devices based on more traditional semiconductors still poses problems when scaling down to few nanometers. These problems are multiscale and multidisciplinary in nature. In the coming years we expect an increasing level of collaboration between industries and research institutions on focused research projects aimed at developing the required knowledge-based infrastructure and enabling predictive simulation power needed to tackle charge transport problems in these materials.

November 5<sup>th</sup> 2014

The Organizers

## 1.2 Program of the International CECAM-Tutorial

”High performance models for charge transport in large scale materials systems”

Bremen Center for Computational Materials Science - BCCMS

University of Bremen, October 5th 6th 2014

Sunday, October 5<sup>th</sup> 2014 (BCCMS, University Campus, TAB Building, Entrance F)

08.00 - 08.30	Registration
08.30 - 10.00	Lecture Benjamin Hourahine, University of Strathclyde, UK <i>Basics of density functional theory</i>
10.00 - 10.30	Coffee Break
10.30 - 12.00	Lecture Blint Aradi, University of Bremen, Germany <i>Density functional tight binding the fast way of doing quantum mechanics</i>
12.00 - 13.00	Lunch Break
13.00 - 15.00	Hands on Session <i>Basic quantum mechanical simulations with the DFTB+ code</i>
15.00 - 15.30	Coffee Break
15.30 - 17.00	Lecture Alessandro Pecchia, The National Research Council ISMN, Rome, Italy <i>Introduction to Equilibrium Greens Functions for electron transport calculations</i>
17.00 - 17.20	Coffee Break
17.20 - 18.30	Hands On Session <i>Equilibrium Greens Function transport calculation with DFTB+ and libNEGF</i>
19.00	Dinner (Restaurant Platzhirsch)



### 1.3 Program of the International CECAM-Tutorial

”High performance models for charge transport in large scale materials systems”

Bremen Center for Computational Materials Science - BCCMS

University of Bremen, October 5<sup>th</sup> 6<sup>th</sup> 2014

Monday, October 6<sup>th</sup> 2014 (BCCMS, University Campus, TAB Building, Entrance F)

08.30 - 10.00 Lecture

Alessandro Pecchia, The National Research Council ISMN, Italy

*Non-Equilibrium Greens Function formalism for transport calculations I*

10.00 - 10.30 Coffee Break

10.30 - 12.00 Hands On Session

*Non-Equilibrium Greens Function transport calculation with DFTB+ and lib-NEGF I*

12.00 - 13.30 Lunch Break

13.30 - 15.00 Lecture

Gabriele Penazzi, University of Bremen, Germany

*Non-Equilibrium Greens Function formalism for transport calculations II*

15.00 - 15.30 Coffee Break

15.30 - 17.00 Hands On Session

*Non-Equilibrium Greens Function transport calculation with DFTB+ and lib-NEGF II*

17.00 - 17.30 Coffee Break

Guest Talks

17.30 - 18.30 Matthias Auf der Maur, University of Rome Tor Vergata, Italy

*Introduction to the multiscale tool TiberCAD*

Guest Talks

18.30 - 19.30 Gerhard Klimeck, Purdue University, West Lafayette, Indiana, US

*Introduction to Nanohub*

## 1.4 Program of the International CECAM-Workshop

”High performance models for charge transport in large scale materials systems”

Bremen Center for Computational Materials Science - BCCMS

University of Bremen, October 6<sup>th</sup> - 10<sup>th</sup> 2014

Tuesday, October 7<sup>th</sup> 2014 (House of Science, Bremen Downtown)

- 08.00 - 08.50 Registration
- 08.50 - 09.00 Opening and welcome, Thomas Frauenheim
- Session: **Tight Binding methods I**  
**Chair: Tim Wehling**
- 09.00 - 09.40 Gerhard Klimeck, Purdue University, West Lafayette, Indiana, US  
*Development of the NEMO tool suite: from basic physics to real industrial devices and to global impact on nanohub.org*
- 09.40 - 10.20 Avik Ghosh, University of Virginia, Charlottesville, US  
*Mixing, matching and stitching - making semi-empirical bandstructures practical yet predictive for transport application*
- 10.20 - 10.50 Coffee Break
- 10.50 - 11.30 Gerd Czycholl, University of Bremen, Germany  
*DC and AC charge transport calculations within empirical tight-binding models*
- 11.30 - 12.10 Mathieu Luisier, Swiss Federal Institute of Technology Zurich, Switzerland  
*Electro-thermal simulations of nanoelectronic devices*
- 12.10 - 14.00 Lunch Break (Restaurant Stadtwirt) and Coffee
- Session: **Tight Binding methods II**  
**Chair: Csar A. Rodrguez Rosario**
- 14.00 - 14.40 Yann-Michel Niquet, Alternative Energies and Atomic Energy Commission, Grenoble, France  
*NEGF modeling of nanodevices: from atomistic tight-binding to k.p perspectives*
- 14.40 - 15.20 Amretashis Sengupta, Indian Institute of Science, Bangalore, India  
*Study of next generation 2-D channel material MOSFETs with empirical tight binding NEGF formalism*
- 15.20 - 15.50 Coffee Break
- 15.50 - 16.30 Oded Hod, Tel Aviv University, Israel  
*A state representation approach for atomistic time-dependent transport calculations in molecular junctions*
- 15.50 - 16.30 Wolfgang Wenzel, Karlsruhe Institute of Technology, Germany  
*A self-consistent first-principles approach model carrier mobility in organic materials*
- 19.00 - 21.30 Welcome Reception (Bremen Town Hall)

## 1.5 Program of the International CECAM-Workshop

”High performance models for charge transport in large scale materials systems”

Bremen Center for Computational Materials Science - BCCMS

University of Bremen, October 6<sup>th</sup> - 10<sup>th</sup> 2014

Wednesday, October 8<sup>th</sup> 2014 (House of Science, Bremen Downtown)

Session:        **Density Functional tight Binding**

**Chair: Thomas Frauenheim**

09.00 - 09.40    Gianaurelio Cuniberti, Dresden University of Technology, Germany

*Quantum transport in nanodevices: orbital-to-continuum models*

09.40 - 10.20    Thomas Heine, Jacobs University, Bremen, Germany

*NEGF-DFTB calculations on charge transport in transition metal dichalco-  
genide nanostructures*

10.20 - 11.00    Benjamin Hourahine, University of Strathclyde, Glasgow, UK

*Magneto-optics and topological materials*

11.00 - 11.30        Coffee Break

11.30 - 12.10    Thomas Niehaus, University of Regensburg, Germany

*Dynamical aspects in quantum transport*

12.10 - 12.50    Guan Hua Chen, University of Hong Kong, China

*Transient current through molecular and nanoscopic devices*

12.50 - 14.30        Lunch Break (Restaurant Stadtwirt) and Coffee

Session:        **Kernel Polynomials**

**Chair: Gerd Czycholl**

14.30 - 15.10    Shengjun Yuan, Radboud University of Nijmegen, The Netherlands

*Large-scale tight-binding simulations of transport and optical properties of two-  
dimensional crystals*

15.10 - 15.50    Stephan Roche, Catalan Institute of Nanosciences and Nanotechnology (ICN2), Barcelona,

*Quantum transport coefficients with real space order-N Kubo-methodologies:  
dissipative component and non-dissipative quantum hall conductivity*

15.50 - 16.20        Coffee Break

16.20 - 17.00    Stanislav Markov, University of Hong Kong, China

*Towards atomic level simulation of electron devices including the  
semiconductor-oxide interface*

17.00 - 17.40    Massimiliano di Ventra, University of California, San Diego, US

*A comparison of different approaches to quantum transport and implications  
for nanoscale systems and cold-atom dynamics*

19.00 - 22.30        Conference Dinner (Restaurant Juergenshof)

## 1.6 Program of the International CECAM-Workshop

”High performance models for charge transport in large scale materials systems”

Bremen Center for Computational Materials Science - BCCMS

University of Bremen, October 6<sup>th</sup> - 10<sup>th</sup> 2014

Thursday, October 9<sup>th</sup> 2014 (University Campus, TAB Building, Main Entrance)

Session: **Multiscale methods I**

**Chair: Guan Hua Chen**

- 09.00 - 09.40 Matthias Auf der Maur, University of Rome Tor Vergata, Italy  
*Approaches to the coupling of FEM and atomistic models for electronic device simulation*
- 09.40 - 10.20 Chi Yung Yam, Beijing Computational Science Research Center, China  
*Multiscale quantum mechanics/electromagnetics method for device simulations*
- 10.20 - 11.00 Alessandro Pecchia, The National Research Council ISMN, Rome, Italy  
*transport in nanoscale materials using the DFTB-NEGF method*
- 11.00 - 11.30 Coffee Break  
textbfChair: Chi Yung Yam
- 11.30 - 12.10 Denis Andrienko, Max Planck Institute Mainz, Germany  
*Design rules for organic semiconductors for optoelectronic applications*
- 12.10 - 12.50 Marcus Elstner, Karlsruhe Institute of Technology, Germany  
*Mixed quantum-classical fragment orbital based non-adiabatic molecular dynamics simulations for charge transfer in complex systems*
- 12.50 - 13.30 Klaus Morawetz, Muenster University of Applied Science, Germany  
*Nonlocal quantum kinetic theory - a method to simulate strong correlations*
- 13.30 - 15.00 Lunch Break (Restaurant Caf Unique) and Coffee

Session: **Multiscale methods II**

**Chair: Marcus Elstner**

- 15.00 - 15.40 Ulrich Kleinekathoefer, Jacobs University, Bremen, Germany  
*Environmental effects on currents through molecular junctions*
- 15.40 - 16.20 Gabriele Penazzi, University of Bremen, Germany  
*Tight Binding modeling of charge transport in disordered materials*
- 16.20 - 17.00 Dmitry Ryndyk, Dresden University of Technology, Germany  
*Modeling of quantum transport at nanoscale: localized molecular orbitals and vibrons*
- 17.00 - 21.00 Poster Session and Catering Buffet

## 1.7 Program of the International CECAM-Workshop

”High performance models for charge transport in large scale materials systems”

Bremen Center for Computational Materials Science - BCCMS

University of Bremen, October 6<sup>th</sup> - 10<sup>th</sup> 2014

Friday, October 10<sup>th</sup> 2014 (University Campus, TAB Building, Main Entrance)

Session:	<b>Ab Initio methods</b>
	<b>Chair: Alessandro Pecchia</b>
09.00 - 09.40	Giovanni Pizzi, Swiss Federal Institute of Technology Lausanne, Switzerland <i>Maximally-localized Wannier functions and their application to the calculation of transport and thermoelectric properties</i>
09.40 - 10.20	Simon M.-M. Dubois, Catholic University of Louvain, Belgium <i>Large scale quantum transport within the optimal basis density matrix minimization approach</i>
10.20 - 10.50	Coffee Break
10.50 - 11.30	Stefano Sanvito, Trinity College Dublin, Ireland <i>Constrained DFT and large scaling: a new pathway to quantitative transport theory</i>
11.30 - 12.10	Csar A. Rodrguez Rosario, University of Bremen, Germany <i>Quantum thermodynamics</i>
12.10 - 12.20	Closing remarks
12.20	Departure

## 1.8 List of Participants

### 1.8.1 Invited Speakers & Chairpersons

- Dr. Denis Andrienko  
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- Prof. Dr. Gerd Czycholl  
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