1 CECAM Tutorial & Workshop

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

October 5^{th} - 10^{th} 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

Contents

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^{th} until October 10^{th}

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-troughput 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 accomodated 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 packeges 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 ermerging 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/SiO2). (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/MoS2, 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^{th} 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^{th} 2014 (BCCMS, University Campus, TAB Building, Entrance F)

08.00 - 08.30		Registration
08.30 - 10.00	Lecture	
		Benjamin Hourahine, University of Strathclyde, UK
		Basics of density functional theory
10.00 - 10.30		Coffee Break
10.30 - 12.00	Lecture	
		Blint Aradi, University of Bremen, Germany
		Density functional tight binding the fast way of doing quantum mechanics
12.00 - 13.00		Lunch Break
13.00 - 15.00	Hands on Session	
		Basic quantum mechanical simulations with the DFTB+ code
15.00 - 15.30		Coffee Break
15.30 - 17.00	Lecture	
		Alessandro Pecchia, The National Research Council ISMN, Rome, Italy
		Introduction to Equilibrium Greens Functions for electron transport calculations
17.00 - 17.20		Coffee Break
17.20 - 18.30	Hands On Session	
		Equilibrium Greens Function transport calculation with DFTB+ and libNEGF
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^{th} 6^{th} 2014

Monday, October 6^{th} 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 libNEGF 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 libNEGF 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^{th} 10^{th} 2014

Tuesday, October 7^{th} 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, Fran
	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

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Bremen Center for Computational Materials Science - BCCMS
University of Bremen, October 6^{th} 10^{th} 2014

Wednesday, October 8^{th} 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 dichalcogenide 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^{th} 10^{th} 2014

Thursday, October 9^{th} 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
	ransport 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^{th} 10^{th} 2014

Friday, October 10^{th} 2014 (University Campus, TAB Building, Main Entrance)

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

1.8 List of Participants

1.8.1 Invited Speakers & Chairpersons

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