Program of the International CECAM-Workshop

"Approximate Quantum Methods in the *ab initio* World"

Beijing Computational Science Research Center, November 08th - November 11th 2016

Tuesday, November 08th 2016 (CSRC Building, 1/F)

17:00 – 20:00 Registration

Wednesday, November 09th 2016 (CSRC Conference Room, 3/F)

08:00 – 08:50 Registration

08:50 – 09:00 Opening and welcome

Session: **DFTB**

Chair: Thomas Frauenheim

09:00 – 09:35 Marcus Elstner, Karlsruhe Institute of Technology, Germany
The approximate DFT models 'DFTB': performance and challenges

09:35 – 10:10 Stefan Irle, University of Nagoya, Japan
Replica exchange MD simulations with linear-scaling density-functional tight-binding

10:10 – 10:45 Julian Kranz, Karlsruhe Institute of Technology, Germany
Linear response time-dependent density functional tight-binding method with a range separated functional

10:45 – 11:25 **Group Photo & Coffee Break**

Session: **Applications-I**

11:25 – 12:00 Kenneth M. Merz, Jr., Michigan State University, USA
Using QM Methods to Refine Biological Structure

12:00 – 12:35 Martin Persson, Dassault Systèmes, Cambridge, UK
Predicting phase stability and mechanical properties of materials

12:35 – 14:30 **Lunch Break** (*Canteen B1/F*)

Session: **Large-scale Molecular Systems**

Chair: Marcus Elstner

14:30 – 15:05 Hiromi Nakai, Waseda University, Japan
Recent Advances of DC-DFTB-K Program

15:05 – 15:40 Tomasz A. Wesolowski, University of Geneva, Switzerland
Describing environment effect on the electronic structure from density embedding methods

15:40 – 16:10 **Coffee Break**

16:10 – 16:45 Alister Page, The University of Newcastle, Australia
Extended Timescale Simulations – Combining Global Reaction Route Mapping and Kinetic Monte Carlo Theory

18:00 – 20:30 **Poster Session** (Pizza & Snacks, *Corridor 3/F*)

Thursday, November 10th 2016 (CSRC Conference Room, 3/F)

Session: **Charge Transport and Dynamics**

Chair: Thomas Niehaus

09:00 – 09:35 GuanHua Chen, The University of Hong Kong, Hong Kong
Alternative Approach to Chemical Accuracy: A Neural Networks-Based First-Principles Method for Heat of Formation of Molecules Made of H, C, N, O, F, S, and Cl

09:35 – 10:10 Alessandro Pecchia, The National Research Council, Rome, Italy
Thermal transport in two dimensional materials

10:10 – 10:45 Stanislav Markov, The University of Hong Kong, Hong Kong
Application of Density Functional Tight Binding to Atomistic Modelling of Field-effect Transistors

10:45 – 11:15 **Coffee Break**

11:15 – 11:50 Oleg Prezhdo, University of Southern California, USA
Nonadiabatic Dynamics of Nanoscale Materials with Tight-Binding DFT

11:50 – 12:25 Sheng Meng, Chinese Academy of Sciences, China,
Atomistic Mechanism and Quantum Selectivity of Plasmon-Induced Water Splitting

12:25 – 14:30 **Lunch Break** (*Canteen B1/F*)

Session: **TD-DFTB and excited states**

Chair: Stanislav Markov

14:30 – 15:05 Thomas Heine, University of Leipzig, Germany
Tight-Binding approximations to TD-DFT

15:05 – 15:40 Thomas Niehaus, University of Regensburg, Germany
Time dependent extension of long-range corrected DFTB

15:40 – 16:10 **Coffee Break**

16:10 – 16:45 Tim Kowalczyk, Western Washington University, USA

Solvation and encapsulation of photoactive species: insights from excited state DFTB

16:45 – 17:20 Cristián G. Sánchez, Ciudad Universitaria, Argentina
Time Dependent Tight Binding Implementation in DFTB+

18:00 – 21:00 **Banquet** (*Chuan Zhe Hui*)

Friday, November 11th 2016 (CSRC Conference Room, 3/F)

Session: **Applications-II**

Chair: Bálint Aradi

09:00 – 09:35 Ben Hourahine, University of Strathclyde, United Kingdom
Correlation of electrons in DFTB

09:35 – 10:10 Henryk Witek, National Chiao Tung University, Taiwan
Automatized parameterization of the DFTB model

10:10 – 10:45 Fernand Spiegelman, CNRS and University of Toulouse, France
Benchmarking DFTB for silver and gold materials: from small clusters to bulk

10:45 – 11:15 **Coffee Break**

11:15 – 11:50 Dongbo Zhang, Beijing Computational Science Research Center, Beijing
Generalized Bloch Theorem and its Application to Low Dimensional Materials

11:50 – 12:25 Jan Rezac, Institute of Organic Chemistry and Biochemistry AS CR, Czech Republic
Correcting DFTB for non-covalent interactions, and its application to drug design

12:25 – 12:35 **Closing remarks**

12:35 – 14:00 **Lunch** (*Canteen B1/F*)

14:00 **Excursion to Summer Palace**