Program of the International CECAM-Tutorial

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

Beijing Computational Science Research Center, November 07th - November 08th 2016

Sunday, November 06th 2016 (CSRC Building, 1/F)

14:00 – 17:00	**Registration**	

Monday, November 07th 2016 (CSRC Conference Room, 3/F)

08:00 – 09:00 **Registration**

09:00 – 11:00 **Tutorial**
Benjamin Hourahine, University of Strathclyde, Glasgow, UK
Bálint Aradi, University of Bremen, Germany

Ground-state properties and molecular dynamics simulations

11:00 – 11:30 **Coffee Break**

11:30 – 12:30 **Commercial demonstration**
Martin Persson, Dassault Systèmes, Cambridge, UK

DFTB in the Materials Studio Suite

12:30 – 14:00 **Lunch Break** (*Canteen B1/F*)

14:00 – 16:00 **Tutorial**
Cristián G. Sánchez, National University of Córdoba, Argentina
Franco Bonafe, National University of Córdoba, Argentina

Absorption spectra and excitations from real time TD-DFTB

16:00 – 16:30 **Coffee Break**

16:30 – 18:30 **Tutorial**
Alessandro Pecchia, The National Research Council, Rome, Italy
Dmitry Ryndyk, TU Dresden, Germany

Modelling charge transport with NEGF-DFTB

18:30 – 20:00 **Dinner** (*Canteen B1/F*)

Tuesday, November 08th 2016 (CSRC Conference Room, 3/F)

09:00 – 11:00   **Tutorial**
Chi Yung Yam, Beijing Computational Science Research Center, China
Stanislav Markov, The University of Hong Kong, China

Modelling of device functions

11:00 – 11:30   **Coffee Break**

11:30 – 12:30   **Tutorial**
Fernand Spiegelmann, CNRS and University of Toulouse, France

Potential energy Surface exploriation/Configuration Interaction with DFTB (deMon-Nano)

12:30 – 14:00   **Lunch Break** (*Canteen B1/F*)

14:00 – 16:00   **Tutorial**
Thomas Niehaus, University of Regensburg, Germany
Adriel Domínguez García, Max Planck Institute, Hamburg, Germany

Excited state properties using linear response TD-DFTB

16:00 – 16:10   **Closing remarks**

18:00 – 19:30   **Dinner** (*Canteen B1/F*)