# Tentative Program of the International CECAM-Tutorial

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

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

Monday, November 07th 2016

**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 and Coffee**

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

*Non-adiabatic Ehrenfest molecular dynamics*

**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*

**19:00 – 20:30** **Dinner**

Tuesday, November 08th 2016

**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** **Commercial demonstration**
Fernand Spiegelmann, University of Toulouse, France

*Configuration interaction within the DFTB framework (deMon-nano)*

**12:30 – 14:00** **Lunch Break and Coffee**

**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**