Monday	11 January 2016

09:00-09:30 Opening remarks
Ludger Wirtz, Local organizer;
Paul Heuschling, Dean of faculty of Science and Technology, University of Luxembourg;
Christiane Kaell, Fonds National de la Recherche

Ferroic materials

09:30-10:00 Jorge Íñiguez *(Luxembourg Institute of Science and Technology, Belvaux, Luxembourg)*
Realistic large-scale simulations of materials with non-trivial lattice-dynamical and electronic properties)

10:00-10:30 coffee break

DFT-functionals

10:30-11:00 Alexandre Tkatchenko *(FHI Berlin, Germany, University of Luxembourg, Luxembourg)*
Electronic Properties of Molecules and Materials with a Self-Consistent Interatomic van der Waals Density Functional)

11:00-11:30 Ngoc Linh Nguyen *(EPFL, Lausanne, Switzerland)*
First-Principles Photoemission Spectroscopy in Molecules and Electronic Structure of Extended Systems from Koopmans-Compliant Functionals

11:30-12:00 Ryotaro Arita *(RIKEN, Japan)*
Density functional theory for plasmon-assisted superconductivity

12:00-14:00 Lunch Break

Coupled-cluster and QMC : learning from chemistry

14:00-14:30 Klaus Doll *(University of Ulm, Germany)*
Extrapolating accurate wave-function based energies from clusters to bulk

14:30-15:00 George Booth *(King's College London, United Kingdom)*
Stochastic quantum chemistry for molecules and solids)

15:00-15:30 Andreas Grüneis *(Max-Planck-Institute for Solid State Research, Stuttgart, Germany)*
Towards Efficient Coupled Cluster Theories for Solids

15:30-16:00 coffee break

Layered Systems

16:00-16:30 Sébastien Lebègue *(Université de Lorraine/CNRS, France)*
New two dimensional compounds: beyond graphene

16:30-17:00 Maria Hellgren *(IMPMC, Paris, France)*
Impact of electronic correlation on the charge density wave instability in TiSe2)

17:00-20:00 Poster session (with light snacks)

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Electron-phonon interaction

09:00-09:30 Matthieu Verstraete *(University of Liège, Belgium)*
Ab initio phonon limited transport

09:30-10:00 Lilia Boeri *(Graz University of Technology, Austria)*
High-pressure hydrides: conventional high-Tc superconductors

10:00-10:30 coffee break

Excited-state dynamics

10:30-11:00 Marco Bernardi *(California Institute of Technology, Pasadena, USA)*
Ultrafast Dynamics of Excited Electrons in Materials

11:00-11:30 Carlo Andrea Rozzi *(CNR, Modena, Italy)*
Ultrafast charge separation dynamics in photovoltaic heterojunctions

11:30-12:00 Federica Agostini *(MPI Halle, Germany)*
Coupled Electron-Nuclear Dynamics in Non-Adiabatic Processes

12:00-14:00 Lunch Break

Green's function methods/ MBPT

14:00-14:30 Michiel van Setten *(UC Louvain, Belgium)*
GW and molecules: a benchmark for G0W0 and developments beyond

14:30-15:00 Manish Jain *(IISC, Bangalore, India)*
Improved quasiparticle wave functions and mean field for G0W0 calculations

15:00-15:30 Eran Rabani *(Department of Chemistry, University of California, Berkeley)*
Stochastic Approaches to Electronic Structure: From DFT and TDDFT to GW and BSE

15:30-16:00 coffee break

Random Phase Approximation

16:00-16:30 Thomas Olsen *(DTU, Denmark)*
Total energy calculations beyond the Random Phase Approximation

16:30-17:00 Dario Rocca *(Université de Lorraine, Vandoeuvre-lès-Nancy, France)*
Dielectric matrix formulation of correlation energies in the Random Phase Approximation: Inclusion of exchange effects

17:45-19:15 Guided walk through the old city of Luxembourg

19:30 Conference dinner

Exploring energy surfaces and phase space (MD)

09:00-09:30 Fabio Pietrucci *(Université Pierre et Marie Curie – Sorbonne, Paris, France)*
A unified approach to reactions in gas phase and solution via topological coordinates

09:30-10:00 Robert Baldock *(University of Cambridge, United Kingdom)*
Calculating the pressure-temperature phase diagrams of materials

Applications of DFT

10:00-10:30 Victor Pardo *(Universidade Santiago de Compostela, Spain)*
Layered iridates: a discussion on noncollinear vs collinear treatment of 5d electron systems

10:30-11:00 Jean-Sébastien Filhol *(Université de Montpellier, Montpellier, France)*
Using the electrochemical dimension for modelling surface and interfaces for energy materials