ESCMQC 2014
September 10-13th 2014, Houffalize, Belgium

Wednesday September 10th

15H00-15H10 : Introduction : Benoît CHAMPAGNE

15H10-16H55
Session 1 : Joop VAN LENTHE

Bernie KIRTMAN

Density functional theory for the response of periodic systems to electric fields based on the vector potential approach

Daniel CRAWFORD

On the non-locality of higher-order molecular properties: A challenge for reduced-scaling models

Gerald KNIZIA

A clean and simple approach to wave function interpretation

16H55-17H15 : Break

17H15-19H00
Session 2 : Jim TALMAN

Frank NEESE

Recent development in pair natural orbital based local coupled cluster methods

Stefan TAUBERT

Magnetically induced ring currents in halogenated benzene molecules using effective core potentials

Christof HÄTTIG

Explicitly correlated coupled cluster methods with pair natural orbitals

19H30 : Dinner

Thursday September 11th

8H30-10H15

Session 3 : Michal JASZUNSKI

Christian OCHSENFELD

Fast quantum-chemical methods for large molecules: from intermolecular interactions to response properties

Lucas VISSCHER

Fast approximations for (TD)-DFT(B)

Sébastien NÉNON

SCC-DFTB as a tool for the study of optoelectronic properties of interfaces

10H15-10H45 : Break

10H45-12H30

Session 4 : Daniel PEETERS

Kenneth RUUD

Analytic calculations of anharmonic effects in vibrational spectroscopy

Fabrizio SANTORO

Recent progresses towards the time-dependent calculation of vibronic spectra of flexible and (or) nonadiabatic systems

Ove CHRISTIANSEN

Tensor decomposition and vibrational coupled cluster theory

12H30-14H30 : Lunch break

14H30-16H50

Session 5 : Dage SUNDHOLM

Mariachiara PASTORE

First principle modelling of structural, optical and charge generation properties of dye/semiconductor heterointerfaces

Frédéric CASTET

Charge separation energetics at organic heterojunctions: on the role of structural and electrostatic disorder

Vincenzo CARRAVETTA

Surface effects in electron photoemission from solutions: cysteine in water

Vincent LIÉGEOIS

Unraveling the vibrational signatures of functionalized surfaces using quantum chemical calculations

16H50-17H20 : Break

17H20-19H30 : Poster session with flash presentations

20H00 : Dinner

Friday September 12th

8H30-10H15
Session 6 : Peter SURJAN

Markus REIHER

The first second-generation DMRG program for quantum chemistry

Sandeep SHARMA

Recent developments in quantum chemistry using matrix product states (MPS)

Sebastian WOUTERS

What can Hartree-Fock theory tell us about the density matrix renormalization group?

10H15-10H45 : Break

10H45-12H30
Session 7 : Antonio RIZZO

Masayoshi NAKANO

Theoretical study on nonlinear optical properties in open-shell singlet molecular systems

Josep M. LUIS

Advances and future prospects in the theoretical evaluation of vibrational nonlinear optical properties

Stefan KNIPPENBERG

An investigation into the (non)linear spectroscopy of small and medium-sized molecules by means of the Algebraic Diagrammatic Construction scheme

12H30-14H30 : Lunch break

14H30-16H15

Session 8 : Christel MARIAN

Chiara CAPPELLI

Modeling solvent effects on molecular properties and spectroscopies: continuum or explicit models?

Daniel ESCUDERO MASA

Multi-determinantal-based DFT studies of the excited state properties of transition metal (TM) complexes

Emmanuel FROMAGER

State-averaged multi-determinant density-functional theory based on ensembles and range separation

16H15-16H45 : Break

16H45-18H30

Session 9 : Alain STRICH

Fred MANBY

Distinguishable cluster theory

Agnes SZABADOS

Geminals with strong orthogonality – varieties, capabilities

Zahid RASHID

A quadratically convergent VBSCF method

19H30 : Dinner and concert

8H30-10H15

Session 10 : Joseph FRIPIAT

Anna KRAWCZUK

From electron density studies towards linear optical properties

Alex TKATCHENKO

From dispersion interactions to farsighted electron correlation – A unified approach based on atomic response functions

Yasutaka KITAGAWA

Theoretical study on electron conductivities of one-dimensional Nickel(II) complexes

10H15-10H45 : Break

10H45-12H30

Session 11 : Daniel P. VERCAUTEREN

Leeor KRONIK

Fundamental and optical gaps from Density Functional Theory

Frank DE PROFT

Reactivity indices from Density Functional Theory: chemistry from the linear response function

David J. TOZER

Molecular binding in post-Kohn–Sham orbital-free DFT

12H30-14H00 : Closure, lunch, and departure