INTERNATIONAL SOLVAY INSTITUTES BRUSSELS

Conceptual Quantum Chemistry: Present Aspects and Challenges for the Future Program (4 - 8 April 2016)

The program consists of a series of invited lectures (35 mins of lecture plus 10 mins of discussion). Also, a total of 10 contributed talks (20 mins of lectures and 5 mins of discussion) are scheduled. On Wednesday evening, a poster session is planned.

MONDAY 4 APRIL

18:00 20:00 Registration and welcome reception

TUESDAY 5 APRIL

9:00 10:00 Registration and coffee

10:00 10:30 Opening session - Frank De Proft and Lode Wyns

Chair 1: Paul Geerlings

10:30 11:15 Gernot Frenking
Molecules With Unusual Bonding Situations - A Challenge for Chemical Bonding Models

11:15 12:00 Alexander Boldyrev
Multicenter Bonding in Chemistry

12:00 13:30 LUNCH

Chair 2: Toon Verstraelen

13:30 14:15 Matthias Bickelhaupt
Theory of chemical bonding and reactivity - Quantitative orbital and activation strain models

14:15 15:00 Israel Fernández
A different approach to understand and control reactivity

15:00 15:45 Ángel Martin Pendás
Some insights into the nature of ground and excited states from real space descriptors

15:45 16:10 Contributed talk: R. Ramakrishnan
Towards reliable electron dynamics across molecular wires and nanostructures

16:10 16:45 COFFEE BREAK

Chair 3: Jeremy Harvey

16:45 17:30 Andreas Savin
Is conceptual chemistry ready to work on open systems?

17:30 18:15 David Cooper
Visual Descriptions of Electronic Structure from Modern Valence Bond Theory: O3 and SO2

WEDNESDAY 6 APRIL

Developments in Conceptual Density Functional Theory: Session in honour of Paul Geerlings

9:00 9:15 Introduction

Chair 4: Kris Van Alsenoy

9:15 10:00 Carlos Cardenas
Chemical response functions in degenerate states and extended systems

10:00 10:30 COFFEE BREAK

10:30 11:15 Alejandro Toro-Labbé
Four concepts to characterize the mechanisms of chemical reactions

11:15 12:00 Patricio Fuentealba
On the concepts of electron donor and electron acceptor systems

12:00 14:00 LUNCH

Chair 5: Anatole von Lilienfeld

14:00 14:45 Paul Ayers
Learning new, and old, chemical concepts from data

14:45 15:30 José Luis Gázquez
Temperature in density functional theory of chemical reactivity

15:30 16:00 COFFEE BREAK

Chair 6: Henri Chermette

16:00 16:25 Contributed talk: Thijs Stuyver
Qualitative insights into molecular transmission: a curly arrow approach

16:25 16:50 Contributed talk: Christophe Morell
Towards the first theoretical scale of the trans effect in octahedral complexes

16:50 17:15 Contributed talk: Andrés Cedillo
Group and fragment electronegativities from constrained SCF methods

17:15 19:15 Poster session

THURSDAY 7 APRIL

Chair 7: Minh Tho Nguyen

9:00 9:45 Miquel Solà
Connecting hydrocarbon and boronhydride chemistries and bidimensional and three-dimensional aromaticities

9:45 10:30 Martin Head-Gordon
Some advances in energy decomposition analysis of electronic structure calculations

10:30 11:00 COFFEE BREAK

Chair 8: Christophe Morell

11:00 11:45 Clémence Corminboeuf
On the many facets of analyzing (non)-covalent interactions

11:45 12:30 Julia Contreras-García
Non covalent interactions: achievements and unsolved challenges of topology

12:30 12:40 Group Photo

12:40 14:00 LUNCH

Chair 9: Laurent Joubert

14:00 14:25 Contributed talk: Roberto Boto
On the topology of the reduced density gradient

14:25 14:50 Contributed talk: Vincent Tognetti
Electron density and reactivity: A synergetic DFT-CDFT-QTAIM approach

14:50 15:15 Contributed talk: Marco Antonio Franco
Beyond the three state ensemble model, Chemical Reactivity Theory for the general case

15:15 15:40 Contributed talk: Steven Vandenbrande
Constructing complete non-covalent force fields based on ab initio monomer densities

15:40 16:05 Contributed talk: Jacek Korchowiec
Application of charge sensitivity analysis to improve the accuracy of the fragmentation based methods of electronic structure calculations

16:05 16:35 COFFEE BREAK

Chair 10: Brian Sutcliffe

16:35 17:20 Arnout Ceulemans
The Symmetry of the Periodic System

17:20 18:05 Eugen Schwarz
The Hidden Physics behind the Periodic Table of Chemical Elements and New Aspects of Valence, Oxidation, Charge and Correlation Numbers

FRIDAY 8 APRIL

Chair 11: to be confirmed

9:00 9:45 Eduard Matito
Characterization and identification of molecular electrides

9:45 10:10 Contributed talk: Mario Van Raemdonck
Constrained CI calculations to investigate charge transfer and the effects of the integer nature of the electron

10:10 10:35 Contributed talk: Stijn De Baerdemaecker
When two is better than one: the seniority scheme as a new tool to build wave functions

10:35 11:00 COFFEE BREAK

Chair 12: to be confirmed

11:00 11:45 Judy Wu
Hydrogen Bond – π-Conjugation Coupling in Enzyme Catalysis: Turning Weak Acids into Strong Proton Donors

11:45 12:00 Closing remarks Patrick Bultinck and lunch