International Symposium 50 years of Quantum Chemistry in Strasbourg

Scientific Program

22-23 November 2019, Collège Doctoral Européen, Université de Strasbourg, Strasbourg, France

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Friday November 22

9:00 Welcome

9:30-10:00 50 years of Quantum Chemistry in 30 mn, **Chantal Daniel** and **Roberto Marquardt**

Chair **Isabella Hyla-Kryspin**

10:00-10:30 OL1 Shin Nakamura, RIKEN Saitama, Japan

Quantum Chemistry and Molecular Science, from LCQ Strasbourg to Practical Researches in Industry, University and National Laboratory. Then Quo Va Dis?

10:30-10:50 Coffee break

10:50-11:10 O1 **Carles Bo**, Institut Catala d'Investigacio Quimica, Spain

Theoretical Studies Towards CO_2 Fixation: 30 years later

11:10-11:30 O2 **Anne Milet**, Université de Grenoble Alpes, France

Theoretical study of the reactivity of complex systems: from biochemical reactions to organic reactions in solution

11:30-11:50 O3 **Ali Kachmar**, Qatar Environment and Energy Research Institute, Qatar

Mapping the free energy landscape of lithium solvation in protic ionic liquids: A metadynamics study

11:50-12:10 O4 **Yann Cornaton**, Université de Strasbourg, France

A noncovalent interaction insight onto the concerted metallation deprotonation mechanism

12:10-12:40 OL2 Robert Moszynski, University of Warsaw, Poland

Two-body and many-body physics in the ultracold regime: a quantum chemist's perspective

12:40 – 14:00 Lunch buffet

Chair **Sergi Vela**

14:00-14:20 O5 **Thierry Leininger**, Univsersité Paul Sabatier, Toulouse, France

The Total Position Spread Tensor as a chemical bond indicator

14:20-14:40 O6 **Houari Brahim**, Université Dr Tahar Moulay-Saida, Algeria

DFT/TD-DFT investigation on the UV-vis absorption and phosphorescence spectra of Pt (II) and Pd (II) complexes with Schiff-base ligands

14:40-15:00 O7 **Antonio Mota**, Universidad de Granada, Spain

Straightening molecular properties ... A chiroptical tale

15:00-15:20 O8 **Mehboob Alam**, University of Calcutta, India

Generalized channel-intereference phenomena in non-linear optical processes

15:20-15:40 O9 **Marie-Catherine Heitz**, Université Paul Sabatier, Toulouse, France

RASPT2 study of the valence excited states of an Fe-porphyrin-carbonyl model complex

15:40 -16:00 O10 **Robert N'Guessan**, Félix Houphouët-Boigny, Abidjan, Ivory Coast

Theoretical and experimental study of alpha-phellandren photodimer isolated in essential oil from monodora myristica

16:00 -16:20 O11 **Emmanuel Fromager**, LCQ, CNRS - Université de Strasbourg, France
Householder transformed density-matrix functional embedding theory

16:20 -17:00 Coffee break

Chair **Vincent Robert**
17:00-18:00 Birth of Quantum Chemistry in Strasbourg in the 60's

17:00 - 17:20 **Jean-Marie Lehn**, Institut de Science et d'Ingénierie Supramoléculaires (ISIS), Université de Strasbourg, France
Birth of Quantum Chemistry in Strasbourg: Alain Veillard, IBMOL and our work - 1968 onwards

17:20 – 18:00 **Alain Dedieu** *Memories*

18:00 – 19:30 Get together for a drink

Saturday November 23

Chair **Nadia Ben Amor**

8:30-9:00 OL3 Josep M. Poblet, Universitat Rovira I Virgili, Tarragona, Spain

Fullerene Cage Selection in Endohedral Metallofullerenes at High Temperatures

9:00-9:20 O12 **Dominique Guillaumont**, INSTN, CEA, Marcoule, France

Actinide ions in solution from experimental and theoretical studies

9:20-9:40 O13 **Ali Rahmouni**, Université Dr Tahar Moulay-Saida, Algeria

Theoretical investigations of cyclic hydrocarbons and nitrogen containing heterocycles in DMSO acidities

9:40-10:00 O14 **Etienne Gindensperger**, LCQ, CNRS - Université de Strasbourg, France

Photo-induced spin-vibronic quantum dynamics

10:00-10:20 O15 **Antonio M. Marquez**, Universidad de Sevilla, Spain

A combinatorial approach for the study of disordered photo-sensitized ferroelectric materials

10:20 – 10:40 Coffee break

Chair **Julien Eng**

10:40-11:00 O17 **Maria Fumanal**, EPFL, Lausanne, Switzerland

Computational Screening of Metal-Organic-Frameworks for Applications in Photocatalysis

11:00-11:20 O18 **Toshiaki Matsubara**, Kanagawa University, Yokohama, Japan
Insight into the Chemical Reactions from the Molecular Dynamics Simulation. How Does the Rare Event Take Place?

11:20-11:40 O19 **Javier Lopez**, Universitat Rovira I Virgili Tarragona, Spain
Understanding Extended Metal Atom Chains: from electronic structure to dynamic behaviour

11:40-12:00 O20 **Bruno Senjean**, Leiden University, The Netherlands
Calculating energy derivatives for quantum chemistry on a quantum computer

12:00 - 13:30 Lunch buffet

Chair **Trond Saue**
13:30-13:50 O21 **Megumi Kayanuma**, AIST, Japan
Mechanisms of Catalytic Reactions

13:50-14:10 O22 **Christophe Gourlaouen**, LCQ, CNRS - Université de Strasbourg, France
Photophysics of Cu(I) complexes: A theoretical study

14:10-14:30 O23 **Radovan Bast**, High Performance Computing Group, UiT Arctic University of Norway, Norway
Coding like it's 1969 - research software engineering recipes for the next two decades

14:30-15:00 OL4 Stefan Knecht, ETH, Zurich, Switzerland
Electronic Structure Theory for the whole Periodic Table of the Elements

15:00-15:30 *The future of Quantum Chemistry in Strasbourg,* **Vincent Robert**