4th International Conference on

PHYSICAL AND THEORETICAL CHEMISTRY

September 18-19, 2017   Dublin, Ireland
Day 1  September 18, 2017
07:00-08:00  Registrations

Redwood Suite B

Keynote Forum

08:10-08:20  Introduction
Title: Excited state lifetimes of isolated iron(ii) complexes and electron injection into TiO$_2$ film
Stefan Haacke, Université de Strasbourg, France

08:20-08:50  Title: Electron/Hole Transformation between Two Atomic Layers
Junrong Zheng, Peking University, China

08:50-09:20  Title: Electrical potential near hydrated solid surface by pH spin probes and labels
Elena G Kovaleva, Ural Federal University

Group Photo
Networking and Refreshments Break 09:50-10:05 @ Redwood Foyer

Sessions:
Physical Chemistry: A Molecular Approach | Physical Chemistry of Macromolecules
Session Chair: Elena G Kovaleva, Ural Federal University, Russia
Session Co-chair: Alex BOEGLIN, Université de Strasbourg, France

10:05-10:25  Title: Sum-frequency generation from chiral bisoxazoline metal complexes: Experiments and dft calculations
Alex BOEGLIN, Université de Strasbourg, France

10:25-10:45  Title: The role of anharmonicity in the confinement effect in zeolites: Structure, spectroscopy and adsorption free energy of ethanol in H-ZSM-5
Roger Rousseau, Pacific Northwest National Laboratory, USA

10:45-11:05  Title: Electron coupling and electron transfer between two bridged dimolybdenum units
Chun Yuan Liu, Jinan University, China

11:05-11:25  Title: Experimental and theoretical studies of coordination fullerene polymers conductivity
Krzysztof Winkler, University of Bialystok, Poland

11:25-11:45  Title: Soft based hypersonic phononics
George Fytas (Talk will be delivered by Yu Cang), Max Planck Institute for Polymer Research, Germany

11:45-12:05  Title: Theoretical study of the chemical reactions by the combination of quantum mechanical and molecular dynamics methods
Toshiaki Matsubara, Kanagawa University, Japan

12:05-12:25  Title: Recent advances in quantum monte carlo: Applications to lithium ion – stockmayer clusters, hydrogen isotopic separation, and the investigation of excited state manifolds
Emanuele Curotto, Arcadia University, USA

12:25-12:45  Title: What is hidden behind a phase diagram?
Fabienne Berthier, Paris-Sud University-CNRS, France

Lunch Break 12:45-13:30 @ Touzai

Sessions: Theoretical and Computational Chemistry | Chemical Physics | Femtochemistry
Session Chair: Vassiliki-Alexandra Glezakou, Pacific Northwest National Laboratory, USA
Session Co-chair: Ivan Štich, Slovak Academy of Sciences, Slovakia

Session Introduction
13:30-13:50  
**Title:** Molecular design strategies for task-specific solvent technologies  
**Vassiliki-Alexandra Glezakou,** Pacific Northwest National Laboratory, USA

13:50-14:10  
**Title:** Magnetism and spin transport in transition metal organometallic clusters  
**Ivan Štich,** Slovak Academy of Sciences, Slovakia

14:10-14:30  
**Title:** Threshold photoelectron and electron-ion coincidence spectroscopies: Past, present and future  
**Richard Tuckett,** University of Birmingham, UK

14:30-14:50  
**Title:** Homogeneous nucleation of solid, liquid and glass phases close to revolution  
**Robert F Tournier,** University of Grenoble, France

14:50-15:10  
**Title:** Recent advances in theoretical spectroscopy from ab initio molecular dynamics  
**Sandra Luber,** University of Zurich, Switzerland

15:10-15:30  
**Title:** Ab initio theory for computing sum frequency generation spectra at aqueous interfaces  
**Tatsuhiko Ohto,** Osaka University, Japan

15:30-15:50  
**Title:** Furious and tranquil radicals: A computational study of sulfur-centred radical chemistry  
**Isa Degirmenci,** Ondokuz Mayis University, Turkey

16:05-16:25  
**Title:** Design of novel imidazole-based corrosion inhibitors - molecular dynamics simulations and electrochemical studies  
**Richard M W Wong,** National University of Singapore, Singapore

16:25-16:45  
**Title:** Fragility of metallic liquids manifest in the high temperature structure and cohesive energy  
**Anup K Gangopadhyay,** Washington University in St. Louis, USA

16:45-17:05  
**Title:** Simulation of DBS, DBS-COOH and DBS-CONHNH$_2$ as hydrogelators  
**Dafna Knani,** ORT Braude College, Israel

17:05-17:25  
**Title:** An appropriate quantum mechanical approach to understand the anomalous behaviors of liquid alkali metals and group-IV alloys  
**Alok Satpathy,** Bir Bikram Memorial College, India

17:25-17:45  
**Title:** Atoms and dimers in rare gas crystals: Modelling of the stable trapping sites  
**Alexei A. Buchachenko,** Skolkovo Institute of Science and Technology, Russia

18:05-18:25  
**Title:** Matrix isolation infrared spectroscopy and structures of weak (O-H···π) and strongly bound (OH···O) binary hydrogen bonded complexes  
**Puja Bani Dev,** Indian Association for the Cultivation of Science, India

18:25-18:45  
**Title:** Determination of the isotopic composition of aqueous solutions radioscopscopic method  
**Rostislav Y Gerasimov,** The Bauman Moscow State Technical University, Russia

18:45-19:05  
**Title:** High-frequency radiations in water under the action of high-voltage short-wave pulses  
**Elchin J. Gurbanov,** Azersu OJSC, Azerbaijan

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**Panel Discussion**

**Day 2 September 19, 2017**

**Redwood Suite B**

**Keynote Forum**

09:00-09:30  
**Title:** Abnormal deformation behavior in a super-soft material: Amorphous zeolite imidazolate framework (a-zif)  
**Wai-Yim Ching,** University of Missouri-Kansas City, USA
09:30-10:00
Title: Non-stoichiometric transition metal oxides: On the interplay of structural complexity, electronic correlations and phonon assisted oxygen ion diffusion
Werner Paulus, University of Montpellier, France

Title: Making headway in understanding the rotation-vibration spectrum of protonated methane \( \text{CH}_3^+ \) - an extremely flexible molecule
Per Jensen, University of Wuppertal, Germany

Networking and Refreshments Break 10:30-10:45 @ Redwood Foyer

Sessions: Photochemistry | Solid-state Chemistry | Spectroscopy | Surface Science | Quantum Chemistry | Biophysical Chemistry
Session Chair: Werner Paulus, University of Montpellier, France
Session Co-Chair: Hideaki Shirota, Chiba University, Japan

Session Introduction

10:45-11:05
Title: Temperature dependent spectral features of room temperature ionic liquids: Aromatic vs. nonaromatic
Hideaki Shirota, Chiba University, Japan

Title: Complex magnetic phases and photo-enhanced ferromagnetism in nano-sized core-shell Prussian blue analogue cubes
Wen-Hsien Li, National Central University, Taiwan

Title: Photoinduced electron transfer through silicon bridge: The source for blue-green emission
Malgorzata Bydla, Adam Mickiewicz University, Poland

Title: Why is gas phase photolysis of 2-nitrophenol a significant source of OH in the polluted atmosphere?
Lei Zhu, University at Albany, USA

Title: Intra- and intermolecular strategies to improving photoluminescence quantum yields of n-π* fluorophores capable of harvesting triplet excitons
Youngmin You, Ewha Womans University, South Korea

Title: A computational investigation of the photochemical oxaziridine conversion process of some experimentally analyzed small-chain conjugated nitrones
Anjan Chattopadhyay, BITS Pilani, India

Title: Topotactic synthesis of mixed-anion oxide epitaxial thin films
Akira Chikamatsu, The University of Tokyo, Japan

Lunch Break 13:05-13:55 @ Touzai

13:55-14:15
Title: On the structure and tribological effect of interfacial water between a graphite surface and metallic or semiconducting counter bodies
Arnaud Caron, KoreaTech - Korea University of Technology and Education, South Korea

Title: Anion and cation diffusion in complex oxides
Manfred Martin, RWTH Aachen University, Germany

Title: New Aspects of an old class of compounds: Tetrelphosphides and their thermoelectric performance
Ulrich Wedig, Max Planck Institute for Solid State Research, Germany

Title: Gold nanoparticles characterization by scattering correlation spectroscopy
Nadia Djaker, Université Paris 13, France

Title: The golden doxorubicin: A tunable design of gold (III)-Doxorubicin complex – PEGylated nanocarrier for oncological Jolanda Spadavecchia, Université Paris 13, France

Title: Particle growth, assembly and extended particle-solvent interactions in deep eutectic solvents
Joshua Hammons, Lawrence Livermore National Laboratory, USA

Networking and Refreshments Break 15:55-16:10 @ Redwood Foyer
PC001
Title: Modelling of electronic spectra of matrix-isolated atoms: Comparison of theoretical approaches
Dmitry S Bezrukov, Skolkovo Institute of Science and Technology, Russia

PC002
Title: Inversion of the lowest singlet excited states induced by the presence of the silicon atom in a styrylcarbazole derivative
Karolina Rachuta, Adam Mickiewicz University, Poland

PC003
Title: Single pulse shock tube investigation of the inter-isomerization and decomposition mechanism of quinoline and isoquinoline. Experimental results and computer simulation
Faina Dubnikova, The Hebrew University of Jerusalem, Israel

PC004
Title: Exciton-mediated electrochemical degradation of blue-phosphorescent organic light-emitting devices
Sinheui Kim, Ewha Womans University, South Korea

PC005
Title: Circularly polarized phosphorescence from cyclometalated Ir(III) complexes having axially chiral ligands
Gyurim Park, Ewha Womans University, South Korea

PC006
Title: Very fast and surprisingly accurate GIAO-mPW1PW91/3-21G//PM7 scaling factor for 13C NMR chemical shifts calculation
Fabio L P Costa, UFG-REJ, Brasil

PC007
Title: Interactions between sodium fire aerosols and fission products- a theoretical chemistry and experimental approach
Ankita Jadon, University of Lille 1, France

PC008
Title: Strongly red-shifted photoluminescence band induced by molecular twisting in cyanine (cy3) dye films
Surendra B Anantharaman, Swiss Federal Laboratories for Materials Science and Technology, Switzerland

PC009
Title: Mechanistic insight towards the activation of aerobic oxidative coupling reactions of alcohols on nanoporous gold
Wilke Dononelli, University of Oldenburg, Germany

PC100
Title: Correlations between structural and optical properties of peroxy bridges from first principles
Blaž Winkler, University of Nova Gorica, Slovenia

PC101
Title: Tolerance factors for organic-inorganic perovskites: Applicability only for high temperature phases
Markus Becker, Carl von Ossietzky University, Germany

PC102
Title: Multiphoto-fragmentation of molecules: REMPI and VMI of HBr
Arnar Hafliðason, University of Iceland, Iceland

PC103
Title: Characterization of protein absorption on gold nanoparticles by scattering correlationspectroscopy
Hanane Moustaoui, Université Paris 13, France

PC104
Title: CHARMM force field and molecular dynamics simulations of polyethylenimine chains
Titus A Beu, Babes-Bolyai University, Romania
Title: Neutron scattering study of super cooled water confined in mesoporous silicas, MCM-41 and SBA-16: Role of component pores and their size
Shigeharu Kittaka, Okayama University of Science, Japan

Title: 57-Fe m"ossbauer spectroscopy on Fe-Mg-O nanocomposite particles grown by a novel chemical vapor synthesis method
Werner Lottermoser, Salzburg University, Austria

Title: In situ hard X-ray photoelectron study of O₂ and H₂O adsorption on Pt nanoparticles
Masaharu Oshima, University of Tokyo, Japan

Title: Pyridinium salts as photoinduced electron traps
R Marshall Wilson, Bowling Green State University, USA

Title: Unpicking vibrational and vibrational torsional couplings in substituted benzenes
Timothy G Wright, University of Nottingham, UK

Title: Reactive surface sites at metal oxide nanoparticles: From fundamental studies to potential medical application
Slavica Stankic, Paris Institute of Nanosciences-CNRS, France

Lunch Break 13:05-13:55 @ Touzai

Title: An embedding technique based on a strategic use of atomic pseudo potentials
Yannick Carissan, Aix-Marseille University, France

Title: Theoretical study of magnetic properties in redox-active ruthenium complexes
Corentin BOILLEAU, Polish Academy of Sciences, Poland

Title: Water interaction and dissociation on the (0001) hematite surface: A DFT+U approach
Fabio R Negreiros, Federal University of ABC, Brazil

Title: Polymer-brush lubrication
Torsten Kreer, Leibniz Institute for Polymer Research Dresden e. V. (IPF), Germany

Title: Excited-state symmetry breaking of linear quadrupolar chromophores: A transient absorption study
Nadia Dozova, Pierre and Marie Curie University, France

Title: Phase equilibrium of the melt-vapor in the tellurium-sulfur system
Valery N Volodin, Institute of Metallurgy and Ore Beneficiation, Kazakhstan

Networking and Refreshments Break 15:55-16:10 @ Redwood Foyer

Bookmark your dates

5th International Conference on

PHYSICAL AND THEORETICAL CHEMISTRY

October 11-13, 2018 | Edinburgh, Scotland