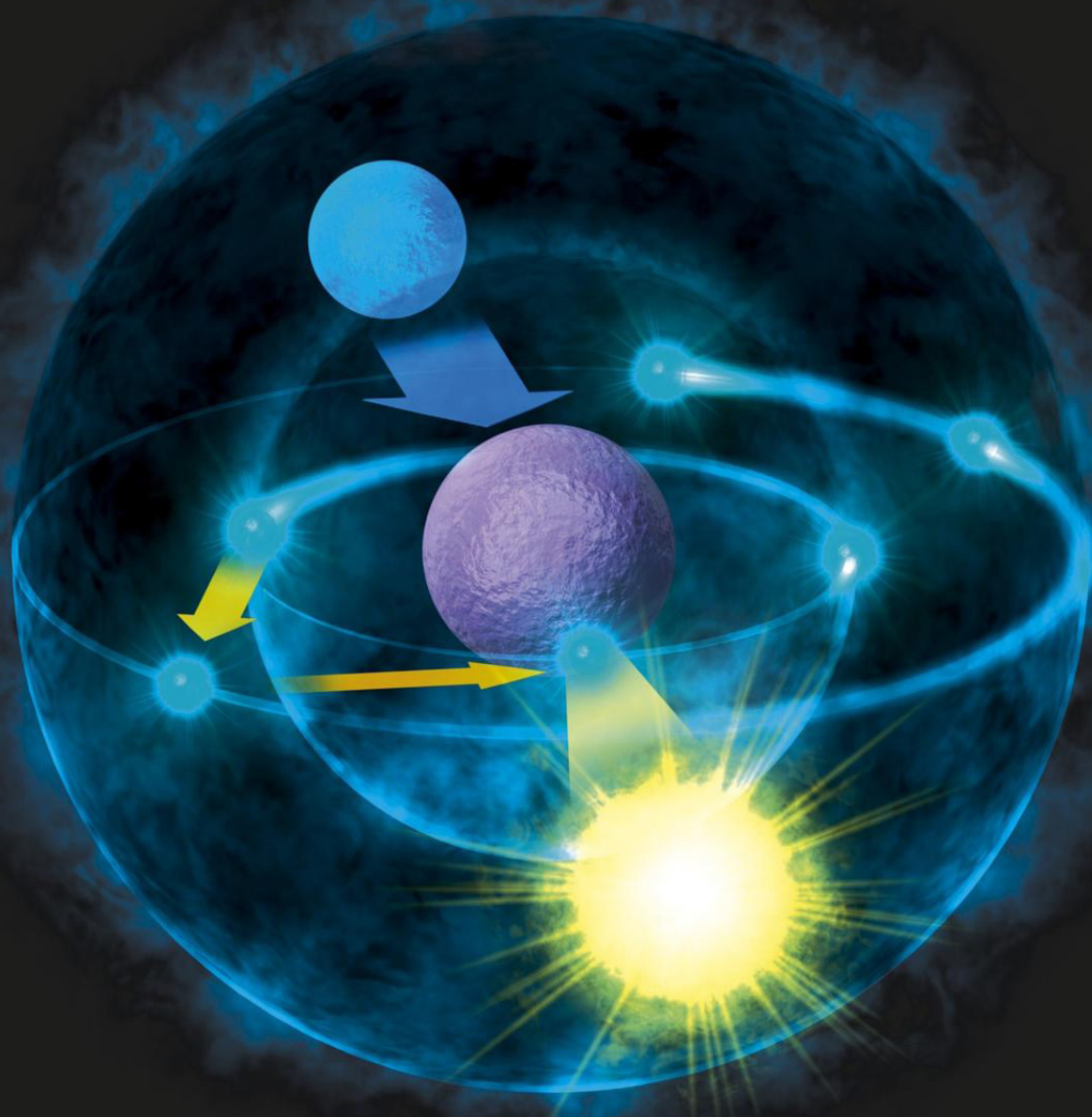


4th International Conference on

PHYSICAL AND THEORETICAL CHEMISTRY

September 18-19, 2017 Dublin, Ireland



Conference Series - America

One Commerce Center-1201, Orange St. #600, Wilmington, Zip 19899, Delaware, USA
Toll Free: 1-888-843-8169, P: 702-508-5200, F: +1-650-618-1417

Conference Series - UK

Kemp House, 152 City Road, London EC1V 2NX, UK
Toll Free: +0-800-014-8923

Redwood Suite B

conference**series**.com 08:00-08:10

Opening Ceremony

Keynote Forum

08:10-08:20 **Introduction**

Title: Excited state lifetimes of isolated iron(ii) complexes and electron injection into TiO₂ film

08:20-08:50

Stefan Haacke, Université de Strasbourg, France

08:50-09:20

Title: Electron/Hole Transformation between Two Atomic Layers

Junrong Zheng, Peking University, China

09:20-09:50

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

Session Introduction

10:05-10:25

Title: Sum-frequency generation from chiral bisoxazoline metal complexes: Experiments and dftcalculations

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 andmolecular 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 Lubner, 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 Mayıs University, Turkey

Networking and Refreshments Break 15:50-16:05 @ Redwood Foyer

- 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: Low energy electrons induced damage to selected dna fragments**
Manabendra Sarma, Indian Institute of Technology Guwahati, India
- 17:05-17:25** **Title: Simulation of DBS, DBS-COOH and DBS-CONHNH₂ as hydrogelators**
Dafna Knani, ORT Braude College, Israel
- 17:25-17:45** **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
- 17:45-18:05** **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 \cdots π) and strongly bound (OH \cdots O) binary hydrogen bonded complexes**
Pujarini Banerjee, Indian Association for the Cultivation of Science, India
- 18:25-18:45** **Title: Determination of the isotopic composition of aqueous solutions radiospectroscopic 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

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 (α -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

10:00-10:30 Title: **Making headway in understanding the rotation-vibration spectrum of protonated methane CH₅⁺ -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

11:05-11:25 Title: **Complex magnetic phases and photo-enhanced ferromagnetism in nano-sized core-shell Prussian blue analogue cubes**

Wen-Hsien Li, National Central University, Taiwan

11:25-11:45 Title: **Photoinduced electron transfer through silicon bridge: The source for blue-green emission**

Malgorzata Bayda, Adam Mickiewicz University, Poland

11:45-12:05 Title: **Why is gas phase photolysis of 2-nitrophenol a significant source of OH in the polluted atmosphere?**

Lei Zhu, University at Albany, USA

12:05-12:25 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

12:25-12:45 Title: **A computational investigation of the photochemical oxaziridine conversion process of some experimentally analyzed small-chain conjugated nitrones**

Anjan Chattopadhyay, BITS Pilani, India

12:45-13:05 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

14:15-14:35 Title: **Anion and cation diffusion in complex oxides**

Manfred Martin, RWTH Aachen University, Germany

14:35-14:55 Title: **New Aspects of an old class of compounds: Tetrelphosphides and their thermoelectric performance**

Ulrich Wedig, Max Planck Institute for Solid State Research, Germany

14:55-15:15 Title: **Gold nanoparticles characterization by scattering correlation spectroscopy**

Nadia Djaker, Université Paris 13, France

15:15-15:35 Title: **The golden doxorubicin: A tunable design of gold (III)-Doxorubicin complex – PEGylated nanocarrier for oncological**

Jolanda Spadavecchia, Université Paris 13, France

15:35-15:55 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

Poster Presentations 16:10-16:25 @ 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

Young Researchers Forum

- 16:25-16:40** **Title: Interactions between sodium fire aerosols and fission products- a theoretical chemistry and experimental approach**
Ankita Jadon, University of Lille 1, France
- 16:40-16:55** **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
- 16:55-17:10** **Title: Mechanistic insight towards the activation of aerobic oxidative coupling reactions of alcohols on nanoporous gold**
Wilke Dononelli, University of Oldenburg, Germany
- 17:10-17:25** **Title: Correlations between structural and optical properties of peroxy bridges from first principles**
Blaž Winkler, University of Nova Gorica, Slovenia
- 17:25-17:40** **Title: Tolerance factors for organic-inorganic perovskites: Applicability only for high temperature phases**
Markus Becker, Carl von Ossietzky University, Germany
- 17:40-17:55** **Title: Multiphoto-fragmentation of molecules: REMPI and VMI of HBr**
Arnar Hafliðason, University of Iceland, Iceland
- 17:55-18:10** **Title: Characterization of protein absorption on gold nanoparticles by scattering correlationspectroscopy**
Hanane Moustouai, Université Paris 13, France

Awards & Closing Ceremony

Break Out @ Fahrenheit Suite

Day 2 September 19, 2017

Sessions: Photochemistry | Solid-state Chemistry | Spectroscopy | Surface Science | Quantum Chemistry | Biophysical Chemistry

Session Chair: Titus A Beu, Babeş-Bolyai University, Romania

Session Co-Chair: Shigeharu Kittaka, Okayama University of Science, Japan

Session Introduction

- 10:45-11:05** **Title: CHARMM force field and molecular dynamics simulations of polyethylenimine chains**
Titus A Beu, Babeş-Bolyai University, Romania

- 11:05-11:25** **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
- 11:25-11:45** **Title: 57-Fe mössbauer spectroscopy on Fe-Mg-O nanocomposite particles grown by a novel chemical vapor synthesis method**
Werner Lottermoser, Salzburg University, Austria
- 11:45-12:05** **Title: *In situ* hard X-ray photoelectron study of O₂ and H₂O adsorption on Pt nanoparticles**
Masaharu Oshima, University of Tokyo, Japan
- 12:05-12:25** **Title: Pyridinium salts as photoinduced electron traps**
R Marshall Wilson, Bowling Green State University, USA
- 12:25-12:45** **Title: Unpicking vibrational and vibrational torsional couplings in substituted benzenes**
Timothy G Wright, University of Nottingham, UK
- 12:45-13:05** **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

- 13:55-14:15** **Title: An embedding technique based on a strategic use of atomic pseudo potentials**
Yannick Carissan, Aix-Marseille University, France
- 14:15-14:35** **Title: Theoretical study of magnetic properties in redox-active ruthenium complexes**
Corentin BOILLEAU, Polish Academy of Sciences, Poland
- 14:35-14:55** **Title: Water interaction and dissociation on the (0001) hematite surface: A DFT+U approach**
Fabio R Negreiros, Federal University of ABC, Brazil
- 14:55-15:15** **Title: Polymer-brush lubrication**
Torsten Kreer, Leibniz Institute for Polymer Research Dresden e. V. (IPF), Germany
- 15:15-15:35** **Title: Excited-state symmetry breaking of linear quadrupolar chromophores: A transient absorption study**
Nadia Dozova, Pierre and Marie Curie University, France
- 15:35-15:55** **Title: Phase equilibrium of the melt-vapor in the tellurium-sulfur system**
Valery N Volodin, Institute of Metallurgy and Ore Benefication, Kazakstan

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

E-mail: physicalchemistry@chemistryconference.org; theoreticalchemistry@chemistryconference.org

Website: physicalchemistry.conferenceseries.com