



Scientific Program

5th International Conference on

Physical and Theoretical Chemistry

October 11- 13, 2018 | Edinburgh, Scotland



UK: Conference Series LLC Ltd
47 Churchfield Road, London, W3 6AY
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DAY-1

October 11, 2018

Meeting Hall: **Macallan Glenfiddich**

08:00-09:00 Registrations

Opening Ceremony **09:00-09:15**

KEYNOTE FORUM

09:15-09:30 Introduction

09:30-10:05 **Title:** Nonadiabatic molecular dynamics following photoexcitation: an *ab initio* quantum approach
Horst Köppel, University of Heidelberg, Germany

10:05-10:40 **Title:** Noncovalent interactions in bio- and nanosciences: quantum mechanical approach
Pavel Hobza, Institute of Organic Chemistry and Biochemistry – CAS, Czech Republic

GROUP PHOTO

Networking & Refreshments 10:40-10:55 @ Academy Lounge

Sessions: Theoretical and Computational Chemistry | Physical Chemistry: A Molecular Approach | Chemical Physics and Chemical Kinetics

Chair: Masahiko Hada, Tokyo Metropolitan University, Japan

Co-Chair: Małgorzata A. Broda, University of Opole, Poland

INTRODUCTION

10:55-11:20 **Title:** Vanadium NMR chemical shift in vanadium complex catalyst: a cooperation of QC calculation and MLR analysis
Masahiko Hada, Tokyo Metropolitan University, Japan

11:20-11:45 **Title:** Experimental and computational studies on the ground state of an isolated Fe(II)-Phthalocyanine
Dana Nachtigallova, Institute of Organic Chemistry and Biochemistry – CAS, Czech Republic

11:45-12:10 **Title:** Quantum chemical study on the tuning thiol-ene polymerization
Isa Degirmenci, Ondokuz Mayıs University, Turkey

12:10-12:35 **Title:** Generalized coordinates hybrid Monte Carlo using high speed robotics algorithms
Laurentiu Spiridon, Institute of Biochemistry of the Romanian Academy, Romania

12:35-13:00 **Title:** Interatomic coulombic decay mediated by ultrafast superexchange energy transfer
Tsveta Miteva, Sorbonne University, France

Lunch Break 13:00-13:45 @ Traders restaurant

13:45-14:10 **Title: A smart strategy for finding global minima of microhydrated biomolecules with minimal DFT calculations**

Kyung Yup Baek, Korea Advanced Institute of Science and Technology, Korea

14:10-14:35 **Title: Atomistic insights into electrochemical interfaces by *ab-initio* simulations and *in-situ* characterizations**

Tadashi Ogitsu, Lawrence Livermore National Laboratory, USA

14:35-15:00 **Title: Structure and spectroscopy of E and Z isomers of Boc-Gly- Δ Phe-NHMe**

Małgorzata A. Broda, University of Opole, Poland

15:00-15:25 **Title: Understanding the non-covalent interaction mediated modulations to the electronic structure of quasi-zero-dimensional graphene nanoflakes**

Amrit Sarmah, Institute of Organic Chemistry and Biochemistry – CAS, Czech Republic

Networking and Refreshments 15:25-15:40 @ Academy Lounge

15:40-16:05 **Title: "Remake" of the non-linear dielectric effect in investigations of structure of liquids**

Kazimierz Orzechowski, University of Wroclaw, Poland

16:05-16:30 **Title: Slowing-down of Pt reduction kinetics in microemulsions: a computer simulation study**

Concha Tojo, University of Vigo, Spain

16:30-16:55 **Title: Modeling reaction kinetics of twin polymerization via differential scanning calorimetry**

Janett Prehl, Chemnitz University of Technology, Germany

16:55-17:20 **Title: The O + O₂ exchange reaction: symmetry, isotope effects, and influence of molecular forces**

Gregoire Guillon, University of Burgundy - Franche-Comté, France

Panel Discussion

DAY-2

October 12, 2018

Meeting Hall: **Macallan Glenfiddich**

KEYNOTE FORUM

09:00-09:35 **Title: Climate change and global warming: thoughts of a quaker scientist**

Richard Tuckett, University of Birmingham, UK

09:35-10:10 **Title: Manipulating liquid crystals via photo generated fields and tailored polymer**

Alexander Lorenz, Paderborn University, Germany

10:10-10:45 **Title: Manipulation of single molecules at surfaces: switches, wires and motors**

Leonhard Grill, University of Graz, Austria

Networking & Refreshments 10:45-11:00 @ Academy Lounge

Sessions: Solid-state Chemistry | Quantum Chemistry | Electro & Photochemistry | Physical Chemistry of Macromolecules

Chair: Alexander Lorenz, Paderborn University, Germany

Co-Chair: Kazimierz Orzechowski, University of Wrocław, Poland

INTRODUCTION

- 11:00-11:25** **Title:** Tuning optical and catalytic properties of ligated noble metal clusters by synergistic role of metallic and organic subunits
Vlasta Bonačić-Koutecký, Humboldt University of Berlin, Germany
- 11:25-11:50** **Title:** Non-isothermal physico-chemical processes in superfluid helium
Eugene B. Gordon, Russian Academy of Sciences, Russia
- 11:50-12:15** **Title:** Versatile approach combining theoretical and experimental aspects of raman spectroscopy to investigate battery materials
Mouna Ben Yahia, ICGM, University of Montpellier, France
- 12:15-12:40** **Title:** Photochemistry of acetohydroxamic acid in solid argon. FTIR and theoretical studies
Magdalena Sałdyka, University of Wrocław, Poland
- 12:40-13:05** **Title:** Excited states deactivation in model proteins chains: nonadiabatic dynamics simulations and *ab initio* methods
Valérie Brenner, Laboratory Interactions, Dynamics and Lasers-CEA Saclay, France

Lunch Break 13:05-13:50 @ Traders restaurant

POSTER PRESENTATIONS 13:50 – 14:20 @ ACADEMY LOUNGE

- PC001** **Title:** Effect of conformational correction to the enthalpy of formation calculated by G4 theory
Taisiya A. Suchkova, Lomonosov Moscow State University, Russia
- PC002** **Title:** Conformational changes in 2-(1,2,4-triazol-3-yl)benzoic acid induced by UV laser light
Magdalena Pagacz-Kostrzewa, University of Wrocław, Poland
- PC003** **Title:** Non-covalently functionalized novel stable complexes of graphene and small molecules
Vijay Madhav Miriyala, Institute of Organic Chemistry and Biochemistry – CAS, Czech Republic
- PC004** **Title:** Prediction of structures of dinucleotide steps containing non Watson-Crick base pairs
Satyabrata Maiti, Saha Institute of Nuclear Physics, India
- PC005** **Title:** Isolated molecule of Iron(II)phthalocyanine exhibits quintet ground-state: a nexus between theory and experiment
Rabindranath Lo, Institute of Organic Chemistry and Biochemistry – CAS, Czech Republic
- PC006** **Title:** Tuning the spin-state of Iron(II)phthalocyanine (FePc) molecules via non-covalent interaction by positioning on functionalized graphene
Debashree Manna, Institute of Organic Chemistry and Biochemistry – CAS, Czech Republic

PC007 **Title: Investigating twin polymerization via density functional theory**

Janett Prehl, Chemnitz University of Technology, Germany

PC008 **Title: Influence of ionic cross-linking on polymer interdiffusion in water-borne pressure-sensitive adhesives**

Hares Wahdat, Clausthal University of Technology, Germany

PC009 **Title: Measurement of dissociation energies for π - π stacked dimers of aromatic hydrocarbons**

Ali Hamzah Alessa, The University of Manchester, UK

SESSIONS

14:20-14:45 **Title: Computational and empiric considerations regarding the electrocatalytic reduction of CO₂ by water soluble cobalt porphyrins**

Yeshayahu Ben-Eliyahu, Ben-Gurion University of the Negev, Israel

14:45-15:10 **Title: Coordination chemistry in pyridine and imidazole compounds containing gem-diol moieties. Solid-state NMR and X-Ray studies**

Juan Manuel Lázaro-Martínez, University of Buenos Aires, Argentina

15:10-15:35 **Title: Surface reactivity of layered manganese oxides: an experimental and theoretical approach**

Germain Vallverdu, University of Pau & Pays Adour, France

Networking & Refreshments 15:35-15:50 @ Academy Lounge

15:50-16:15 **Title: Synthesis and cyclic voltammetry study of asymmetrical triphenylmethane di- and trisulfides on coated and bare gold electrodes**

Imad Ali Abu-Yousef, American University of Sharjah, UAE

SESSIONS

16:15-16:40 **Title: Multiple interacting collective modes and phonon gap in phospholipid membranes**

Giovanna D'Angelo, University of Messina, Italy

16:40-17:05 **Title: Dynamical and structural characterization of thermally responsive pluronic-based nano-delivery systems**

Caterina Branca, University of Messina, Italy

17:05-17:30 **Title: Transition metal systems: a theoretical modeling of their L_{2,3}-edge X-ray absorption spectra**

Silvia Carlotto, University of Padova, Italy

YOUNG RESEARCH FORUM

17:30-17:45 **Title: Application of combined electrochemical reactions for extraction of metals from metal-containing waste**

Sharipov Rustam Hasanovich, Kazakh-British Technical University, Republic of Kazakhstan

17:45-18:00 **Title: Composition for reducing the pour point of diesel fuel**

Myrzakhanov Maxat Makhmudovich, Kazakh-British Technical University, Republic of Kazakhstan

Panel Discussion
Poster Awards Ceremony

DAY-3

October 13, 2018

Networking Session 13:00-14:00 @ Traders restaurant

Closing Ceremony

Bookmark your Dates

6th International Conference on

Physical and Theoretical Chemistry

September 09-10, 2019 | Zurich, Switzerland

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