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7th International Conference on
Physical and Theoretical Chemistry

October 07-08, 2020
Vienna, Austria



SCIENTIFIC PROGRAM



DAY 1
Wednesday, 07th October

08:30-09:00 **Registrations**

09:00-09:30 **Introduction**

09:30-09:50 COFFEE BREAK

09:50-11:50 Meeting Hall 01 **KEYNOTE LECTURES**

11:50-13:10

MEETING HALL 01	MEETING HALL 02
Talks On: Theoretical and Computational Chemistry	**Talks On: Physical Chemistry of Macromolecules**
Theoretical Chemical Kinetics	Complex Compounds
Molecular Modelling	Chemical Thermodynamics
Molecular Mechanics	Electrolysis
Cheminformatics	Physical Chemistry of Plasma
Molecular Dynamics	Potentiostat and Its Applications

13:10-13:15 GROUP PHOTO

13:15-14:00 LUNCH BREAK

14:00-16:00

MEETING HALL 01	MEETING HALL 02
Talks On: Chemical Physics	**Talks On:** Chemical Kinetics
Electromagnetism	Rate of Chemical Reaction
Nuclear and Particle Physics	Integrated Rate Equation
Atomic Systems	Collision Theory
Quantum Mechanics and Symmetry	Temperature Dependence of Reaction
Coordination Chemistry	Order and Molecularity of Reaction
Superconductivity	Catalysts

16:00-16:20 COFFEE BREAK

MEETING HALL 01 (16:20-17:00)	MEETING HALL 01 (17:00-18:00)
Young Researchers	Workshop

DAY 2
Thursday, 08th October

09:00-10:30 Meeting Hall 01 — **KEYNOTE LECTURES**

10:30-10:50 COFFEE BREAK

10:50-12:50	MEETING HALL 01	MEETING HALL 02
	Talks On: Surface Science	**Talks On: Spectroscopy**
	Surface Characterisation and Metrology	Electromagnetic Radiation and Its Interactions
	Nanoscale Tribology	Molecular Symmetry
	Surface Imaging & Depth Profiling	Mass Spectrometry
	Surface Integrity	Vibrational Spectroscopy
	Lubrication and Lubricants	Rotational Spectroscopy
	Coatings and Surface Treatments	Polymer technology

12:50-13:35 LUNCH BREAK

13:35-15:55	MEETING HALL 01	MEETING HALL 02
	Talks On: Photochemistry	**Talks On: Quantum Chemistry**
	Photoelectrochemical Cell	Photonics and Non-linear Optics
	Fluorescence and Phosphorescence	QM/MM Calculations and Solvation Models
	Photochemical Reactions and Their Kinetics	Quantum Monte-Carlo
	Photoelectric Effect	Reaction Mechanisms and Rates
	Photoelectrochemistry	Density Functional Theory
	Photoprocesses	Electron Scattering

15:55-16:15 COFFEE BREAK

MEETING HALL 01 (16:15-17:00)	MEETING HALL 01 (17:00-18:00)
Poster Presentations	Workshop

PAST AFFILIATES

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Horst Köppel
University of Heidelberg, Germany

Pavel Hobza
Institute of Organic Chemistry and Biochemistry – CAS, Czech Republic

Masahiko Hada
Tokyo Metropolitan University, Japan

Dana Nachtigallová
Institute of Organic Chemistry and Biochemistry – CAS, Czech Republic

Isa Degirmenci
Ondokuz Mayis University, Turkey

Laurentiu Spiridon
Institute of Biochemistry of the Romanian Academy Romania

Tsveta Miteva
Sorbonne University, France

Kyung Yup Baek
Korea Advanced Institute of Science and Technology Korea

Tadashi Ogitsu
Lawrence Livermore National Laboratory, USA

Małgorzata A. Broda
University of Opole, Poland

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

Kazimierz Orzechowski
University of Wroclaw, Poland

Concha Tojo
University of Vigo, Spain

Janett Prehl
Chemnitz University of Technology, Germany

Gregoire Guillon
University of Burgundy - Franche-Comté, France

Richard Tuckett
University of Birmingham, UK

Alexander Lorenz
Paderborn University, Germany

Leonhard Grill
University of Graz, Austria

Vlasta Bonačić-Koutecký
Humboldt University of Berlin, Germany

Eugene B. Gordon
Russian Academy of Sciences, Russia

Mouna Ben Yahia
ICGM, University of Montpellier, France

Magdalena Sałdyka
University of Wrocław, Poland

Valérie Brenner
Laboratory Interactions, Dynamics and Lasers-CEA Saclay, France

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

PAST AFFILIATES

Juan Manuel Lázaro-Martínez
University of Buenos Aires, Argentina

Germain Vallverdu
University of Pau & Pays Adour, France

Giovanna D'Angelo
University of Messina, Italy

Caterina Branca
University of Messina, Italy

Silvia Carlotto
University of Padova, Italy

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

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

PAST AFFILIATES

Glimpses of Physical Chemistry Conferences













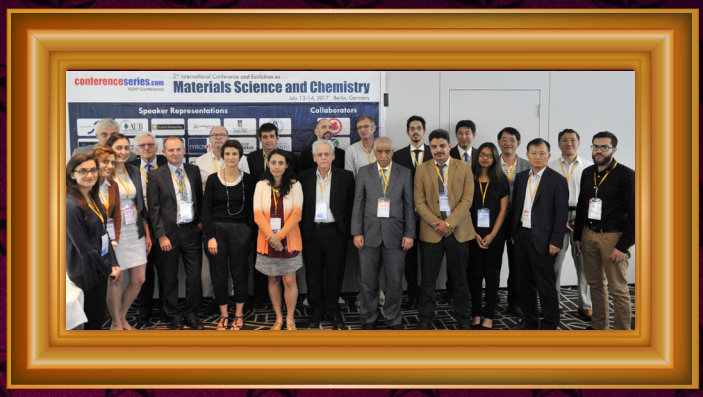




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Glimpses of Physical Chemistry Conferences

















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Vienna Attractions



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

Registrations

Opening Ceremony

KEYNOTE FORUM

Introduction

Title: Nonadiabatic molecular dynamics following photoexcitation: an *ab initio* quantum approach

Horst Köppel, University of Heidelberg, Germany

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 @ 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

Title: Vanadium NMR chemical shift in vanadium complex catalyst: a cooperation of QC calculation and MLR analysis

Masahiko Hada, Tokyo Metropolitan University, Japan

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

Title: Quantum chemical study on the tuning thiol-ene polymerization

Isa Degirmenci, Ondokuz Mayis University, Turkey

Title: Generalized coordinates hybrid Monte Carlo using high speed robotics algorithms

Laurentiu Spiridon, Institute of Biochemistry of the Romanian Academy, Romania

Title: Interatomic coulombic decay mediated by ultrafast superexchange energy transfer

Tsveta Miteva, Sorbonne University, France

Lunch Break @ Traders restaurant

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

Title: Atomistic insights into electrochemical interfaces by *ab-initio* simulations and *in-situ* characterizations
Tadashi Ogitsu, Lawrence Livermore National Laboratory, USA
Title: Structure and spectroscopy of E and Z isomers of Boc-Gly-ΔPhe-NHMe
Małgorzata A. Broda, University of Opole, Poland
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 @ Academy Lounge

Title: "Remake" of the non-linear dielectric effect in investigations of structure of liquids
Kazimierz Orzechowski, University of Wroclaw, Poland
Title: Slowing-down of Pt reduction kinetics in microemulsions: a computer simulation study
Concha Tojo, University of Vigo, Spain
Title: Modeling reaction kinetics of twin polymerization via differential scanning calorimetry
Janett Prehl, Chemnitz University of Technology, Germany
Title: The O + O_2 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

Title: Climate change and global warming: thoughts of a quaker scientist
Richard Tuckett, University of Birmingham, UK
Title: Manipulating liquid crystals via photo generated fields and tailored polymer
Alexander Lorenz, Paderborn University, Germany
Title: Manipulation of single molecules at surfaces: switches, wires and motors
Leonhard Grill, University of Graz, Austria

Networking & Refreshments @ 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 Wroclaw, Poland

INTRODUCTION

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
Title: Non-isothermal physico-chemical processes in superfluid helium
Eugene B. Gordon, Russian Academy of Sciences, Russia
Title: Versatile approach combining theoretical and experimental aspects of raman spectroscopy to investigate battery materials
Mouna Ben Yahia, ICGM, University of Montpellier, France
Title: Photochemistry of acetohydroxamic acid in solid argon. FTIR and theoretical studies
Magdalena Sałdyka, University of Wrocław, Poland
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 @ Traders restaurant

POSTER PRESENTATIONS @ 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

Title: Computational and empiric considerations regarding the electrocatalytic reduction of CO_2 by water soluble cobalt porphyrins
Yeshayahu Ben-Eliyahu, Ben-Gurion University of the Negev, Israel
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
Title: Surface reactivity of layered manganese oxides: an experimental and theoretical approach
Germain Vallverdu, University of Pau & Pays Adour, France

Networking & Refreshments @ Academy Lounge

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

Title: Multiple interacting collective modes and phonon gap in phospholipid membranes
Giovanna D'Angelo, University of Messina, Italy
Title: Dynamical and structural characterization of thermally responsive pluronic-based nano-delivery systems
Caterina Branca, University of Messina, Italy
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

Title: Application of combined electrochemical reactions for extraction of metals from metal-containing waste
Sharipov Rustam Hasanovich, Kazakh-British Technical University, Republic of Kazakhstan
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 @ Traders restaurant

Closing Ceremony