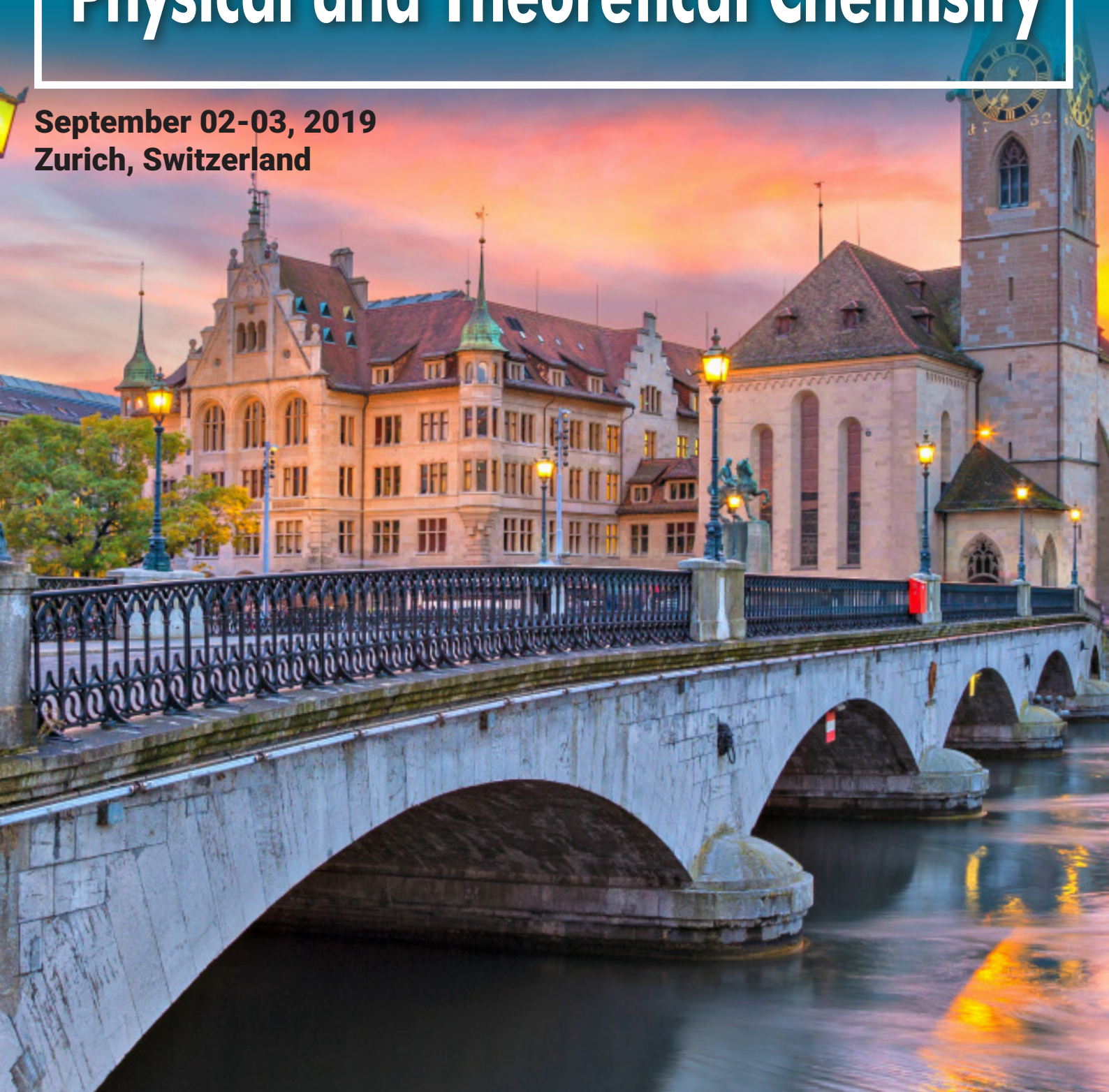


6th International Conference on **Physical and Theoretical Chemistry**

September 02-03, 2019
Zurich, Switzerland



S C I E N T I F I C P R O G R A M

Monday, 02nd September08:30-09:00 **Registrations**09:00-09:30 **Introduction****09:30-09:50 COFFEE BREAK**09:50-11:50
Meeting Hall 01**KEYNOTE LECTURES**

	MEETING HALL 01	MEETING HALL 02
11:50-13:10	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**

	MEETING HALL 01	MEETING HALL 02
14:00-16:00	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)****Young Researchers****MEETING HALL 01 (17:00-18:00)****Workshop**

09:00-10:30
Meeting Hall 01

KEYNOTE LECTURES

10:30-10:50 COFFEE BREAK

	MEETING HALL 01	MEETING HALL 02
10:50-12:50	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

	MEETING HALL 01	MEETING HALL 02
13:35-15:55	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

09:00-10:30
Meeting Hall 01

KEYNOTE LECTURES

10:30-10:50 COFFEE BREAK

	MEETING HALL 01	MEETING HALL 02
10:50-12:50	Talks On: Solid-state Chemistry	Talks On: Biophysical Chemistry
	Condensed Matter Physics	Genomic Biophysics
	Colloids	Physical Chemistry with Applications to the Life Sciences
	Solid State Synthesis	Molecular Imaging
	Diffraction Techniques	Bioelectrochemistry: Fundamentals, Applications and Recent Developments
	Structural Chemistry	Magnetic phenomena
	Catalysis	Plastics fabrication and uses

12:50-13:35 LUNCH BREAK

	MEETING HALL 01	MEETING HALL 02
13:35-15:55	Talks On: Electrochemistry	Talks On: Organometallic Chemistry
	Batteries	Polymers
	Electrolytic Cell	Fullerene
	Deniell Cell	Heterocyclic Compounds
	Concentration Cells	Organometallic Chemistry
	Kohlarusch's Law	Transition Metal Compounds
	Electrode Potential	Industrial organic Chemistry
	Faradays Laws of Electrolysis	Aliphatic and Aromatic Compounds

15:55-16:15 COFFEE BREAK

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

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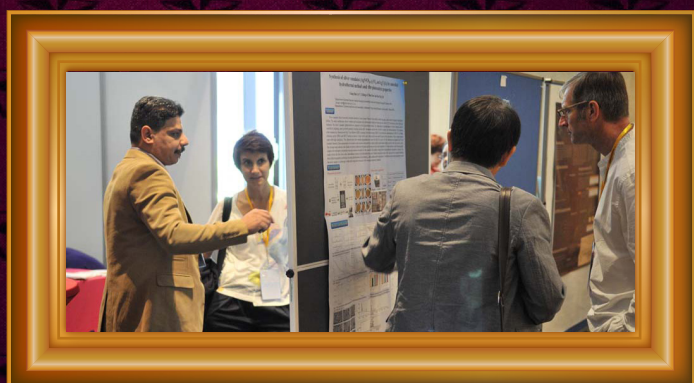
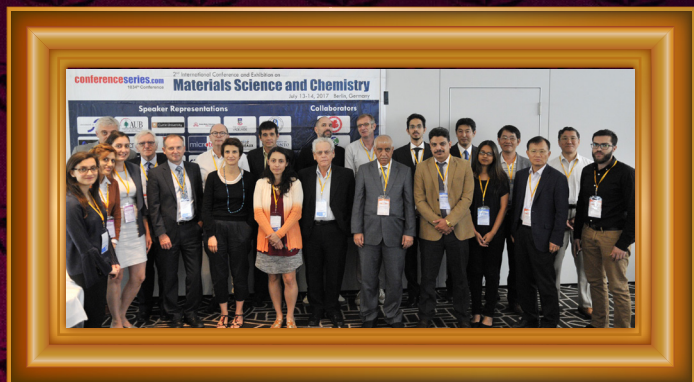
*Kazakh-British Technical University, Republic of
Kazakhstan*

PAST AFFILIATES

Glimpses of PHYSICAL CHEMISTRY Conferences



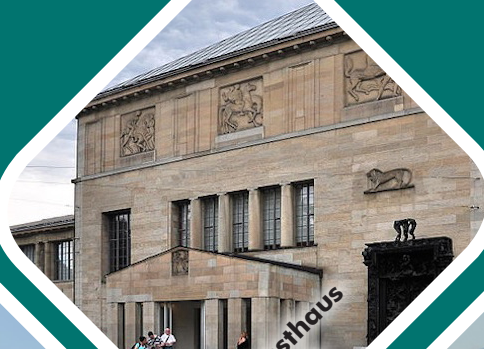
Glimpses of PHYSICAL CHEMISTRY Conferences



Zürich Attractions



Grossmünster



Kunsthaus Zurich



Bahnhofstrasse



Fraumünster



Lake Zurich



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5th International Conference on

Physical and Theoretical Chemistry

October 11- 13, 2018 | Edinburgh, Scotland



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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 Mayıs 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 Wrocław, 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 + 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

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 Wrocław, 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 CO₂ 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