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29.08 - 1.09 2023
Warsaw, Poland

The 6th Quantum Bio-Inorganic Chemistry Conference

qbicvi.sciencesconf.org

The 6th Quantum Bio-Inorganic Chemistry Conference

29.08.23 - 01.09.23
Warsaw, Poland

Organisers

IChF Institute of Physical Chemistry PAS

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Adam Kubas
Institute of Physical Chemistry, Polish Academy of Sciences
Ragnar Björnsson
French Alternative Energies and Atomic Energy Commission (CEA)

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Welcome to QBIC VI!

Dear Colleagues,

We welcome you in Warsaw for the 6th Quantum Bio-inorganic Chemistry Conference (QBIC VI).

The field of quantum (bio)inorganic chemistry continues to evolve as new theoretical methods make an impact, new metalloproteins are discovered, and new avenues of bioinspired chemistry are uncovered. These developments will be covered in our extensive program. Keeping our theoretical field grounded by a close connection to the experiment, we continue the QBIC tradition of inviting experimental scientists. Emerging methodologies, such as quantum computing or machine learning, may change our field completely one day, and you will hear talks on these topics during the conference as well.

QBIC VI takes place in the capital city of Poland, at the Institute of Physical Chemistry, Polish Academy of Sciences (IChF). IChF, located in the Wola district of Warsaw, is the leading research institution dealing with various aspects of chemistry. Funded in 1955, it is among the best scientific units in Poland. The interdisciplinary nature of QBIC meetings aligns very well with the Institute's profile, and IChF supported us at every step in the conference preparation. Moreover, the participants from all around the world, the international scientific committee, and Polish-French-Icelandic organizing team make this conference a truly international experience.

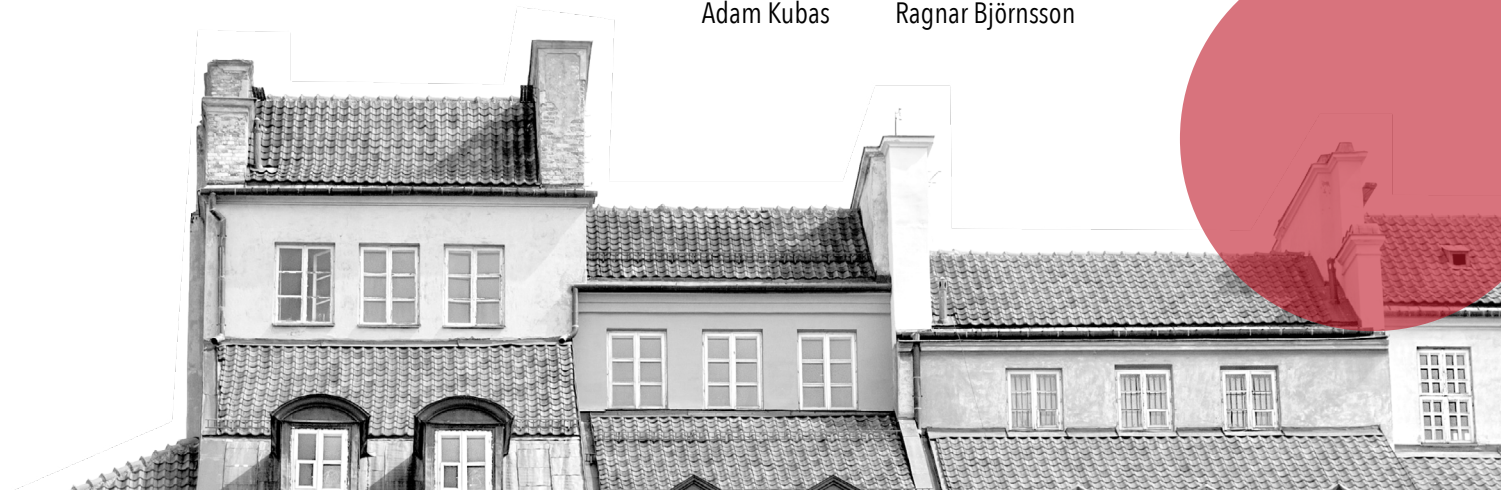
In organizing the program of QBIC VI we followed in the footsteps of the recent successful meetings in Bath (QBIC IV, 2018) and Marseille (QBIC V, 2019). The program features two plenary talks, 6 keynotes, 16 invited talks and 17 contributed oral presentations. In addition, 27 posters will be presented during the poster session.

We hope you will have a great time here discussing the latest ongoing research in our field, starting new collaborations, meeting up with old friends, and making new ones.

On behalf of the scientific and organizing committees,

Adam Kubas

Ragnar Björnsson



QBIC-VI

Book of Abstracts

Read the full abstracts of presentations and posters:

http://doi.org/10.6084/m9.figshare.23996808

Program

Tuesday

29.08

11:00
Adam Kubas,
Institute of Physical Chemistry, Polish Academy of Sciences
Ragnar Björnsson,
French Alternative Energies and Atomic Energy Commission (CEA)
Opening

11:05
Representative of the French Embassy
Welcome word from the Honorary Patron

P **11:10**
Pavel Jungwirth,
Institute of Organic Chemistry and Biochemistry of the Czech Academy of Sciences
Electrons in Polar Solvents: Birch Reduction, Blue Electrolytes, and Golden Metals

K **12:00**
Elżbieta Gumienna-Kontecka,
University of Wrocław
Harnessing the power of siderophore mimics for molecular imaging applications

12:40
Luca Bertini,
University of Milano-Bicocca
Differences and similarities between fungal and bacterial laccases in oxidation of polycyclic aromatic hydrocarbons

13:00
Agnieszka Stańczak,
Institute of Organic Chemistry and Biochemistry, CAS
Unraveling tyrosinase ortho-hydroxylation reaction mechanism: Interplay between experiment and theory

13:20
Lunch break

I **14:40**
Matthias Stein,
Max Planck Institute for Dynamics of Complex Technical Systems Molecular Simulations and Design
Bio-inspired Catalysis and Therapeutics

I **15:10**
Martin Srnec,
J. Heyrovský Institute of Physical Chemistry
Off-diagonal thermodynamics and its effect on reactivity

15:40
Gunasekaran Velmurugan,
Heidelberg University
A dicopper(II)-based carbonic anhydrase model – quantum-chemical evaluation of the mechanistic pathway

16:00
Josep María Luis,
University of Girona
Carboxylic Acid Directed γ -Lactonization of Unactivated Primary C—H Bonds Catalyzed by Mn Complexes

16:20
Erna K. Wieduwilt,
University of Southern Denmark
Exploring off-path reactions of lytic polysaccharide monooxygenases

I **16:40**
Dimitrios Pantazis,
Max Planck Institut für Kohlenforschung
Computational Insights into Ascorbate Peroxidase Compound II

17:10
BBQ

Wednesday

30.08

Speakers:
K Keynote P Plenary I Invited

K **08:30**
Martin Kaupp,
TU Berlin
New DFT approaches beyond the zero-sum game

I **09:10**
Mariusz Radoń,
Jagiellonian University
Experiment-Derived Benchmark Set of Transition Metal Spin-State Energetics for Assessment of Quantum Chemistry Methods

I **09:40**
Katharina Bogusławski,
Nicolaus Copernicus University
Alternative wave function ansätze for (in) organic chemistry

10:10
Coffee break

10:40
Justin Joyce,
Max Planck Institute for Chemical Energy Conversion
Electronic Structure Impact of Nitrogenase's Central Carbide: A QM/MM Study

11:00
Bettina Lier,
University of Natural Resources and Life Sciences Vienna, Institute of Molecular Modeling and Simulation
BuRNN: Machine Learning for Polarizable QM/MM Simulations

I **11:20**
Marcel Swart,
ICREA, IQCC (Universitat de Girona)
Pushing the Limits of Quantum Mechanics in Predicting BioInorganic Reactivity

K **11:50**
Robert Izsak,
Riverlane Research Ltd.
Prospects of Quantum Computational Chemsitry

12:30
Lunch break

13:50
Maylis Orio,
CNRS, Aix Marseille University
Decoding LPMO structures by Theoretical EPR Spectroscopy

14:20
Erik Donovan Hedegård,
University of Southern Denmark
Treating transition metals in solvents and proteins properly

14:40
Esma Birsen Boydas,
Humboldt Universität Berlin
The Good, the Bad, and the Ugly of multiplet dominated X-ray processes

I **15:00**
Hélène Jamet,
University of Grenoble
Theoretical studies of reactive copper-oxygen species

15:30
Rongzhen Liao,
Huazhong University of Science and Technology
QM and QM/MM Studies of Selectivities in Metalloenzymes

15:50
Coffee break

program continues on the next page ▶

Wednesday

30.08

I **16:20**
Tomasz Borowski,
Jerzy Haber Institute of Catalysis and Surface Chemistry PAS
Computational and experimental studies on selected non-heme iron enzymes

16:50
Per Siegbahn,
Stockholm University
Important redox reactions in nature

17:10–19:30
Poster session

Thursday

31.08

P **08:30**
Jochen Blumberger,
University College London
Probing Currents of Bacterial Life with Photochemistry, Scanning Tunneling Microscopy and Computation

K **09:20**
Christophe Léger,
CNRS
Outer-sphere effects in hydrogenase catalysis: a challenge for theoretical chemists?

10:00
Maria Drosou,
Max-Planck-Institut für Kohlenforschung
Insights into the Mechanism of NiFe-Hydrogenase Using Correlated Wavefunction Methods

10:20
Coffee break

I **10:50**
Maren Podewitz,
TU Wien
Catalysis in Confinement: Reaction Mechanism of C-X Coupling with a Cu-calix[8]arene Catalyst

program continues on the next page

Thursday

31.08

Speakers:

K Keynote P Plenary I Invited

11:20
Kyung-Bin Cho,
Jeonbuk National University
Biomimetic inorganic compounds with DFT: some examples

11:40
Ravi Kumar,
Max Planck Institute for Dynamics of Complex Technical Systems
Oxidizing Ni or Fe in the Glutamate Coordinated O2-Tolerant [NiFe]-Hydrogenase: Broken-Symmetry DFT Exploration

I **12:00**
Vijay Gopal Chilkur,
Aix-Marseille University
Discussion of the electronic structure of Iron-Sulfur molecules: ab initio study and model Hamiltonians

12:30
Lunch break

K **13:50**
Karin Fink,
Karlsruhe Institute of Technology
Calculations on the magnetic properties of transition metal and lanthanide compounds

I **14:30**
Nuno Bandeira,
University of Lisbon
Assessing charge transfer and non-innocent ligand character in a low valent nickel complex

I **15:00**
Zdenek Futera,
University of South Bohemia
Electron Tunneling or Hopping? Transport Mechanisms in Protein Junctions Investigated by DFT

15:30
Hossein Jooya,
MathWorks
MATLAB session: Deep Learning from Atoms in Molecules

16:30
QBIC Society meeting

19:30
Dinner

Friday

01.09

Speakers:

K Keynote P Plenary I Invited

K **08:30**
Ryde Ulf,
Lund University
Computational studies of nitrogenase

I **09:30**
Vera Krewald,
TU Darmstadt
The Photochemistry of Azides

I **09:40**
Joanna Kargul,
University of Warsaw
Nanoengineering electron transfer pathways in biomolecular systems for efficient solar conversion

10:10
Coffee break

I **10:40**
Michael Römelt,
Humboldt University
Revealing Complex Electronic Distributions in Transition Metal Compounds with Multireference Electronic Structure Methods

11:10
Cina Foroutan-Nejad,
Institute of Organic Chemistry PAS
Electron in a box; a room-temperature-stable electride

11:30
Marc Reimann,
Technical University Berlin
Optical Excitations of 3d Transition Metal Hexaaqua Complexes – A Challenge for Theory

11:50
Adam Šrut,
Technical University Darmstadt
Quantification of the nuclear coordinates for electron transfer: the antisymmetric and symmetric dimensions of the Marcus–Hush model

Posters

P1
Kosala Amarasinghe,
Leibniz Institute for Catalysis (LIKAT)
Computational Study of Non-Heme Iron Enzymes with Taurine and Hyoscyamine

P2
Tomasz Bednarek, Alexandra Siklitskaya
Institute of Physical Chemistry PAS
Improving the precision of quantum-chemical calculations by novel embedding scheme including Friedel oscillations

P3
Nour El Houda Bensiradj
DFT studies of chemical and biological reactivities of complexes of copper and cobalt with paracetamol as ligand

P4
Priyam Bharadwaz,
J. Heyrovsky Institute of Physical Chemistry, CAS
Reactivity factors in catalytic methanogenesis and their tuning upon coenzyme F430 biosynthesis

P5
Maria Bzowka, Katarzyna Szleper,
Silesian University of Technology
Studying the molecular basics of TLR8 Z-loop proteolytic cleavage by furin protease with an emphasis on the role of water molecules in the system

P6
Anna Cholewinska,
Universitat Rovira i Virgili
Revealing Catalyst's Secrets: the Impact of Substituents in Zinc(II) Complexes with N4-donor ligands on their catalytic performance

P7
Janko Civic,
KU Leuven
Understanding Substrate Binding and Reactivity of Stearoyl-CoA Desaturase (SCD1) through Classical and Multiscale Molecular Dynamics Simulations

P8
Wenhao Deng, Liao Rongzhen
Huazhong University of Science and Technology
Theoretical Study of Selectivities in Sequential Methylations Catalyzed by the B12-dependent SAM radical enzyme TokK

P9
Agnieszka Drzewiecka-Matuszek,
Jerzy Haber Institute of Catalysis and Surface Chemistry PAS
DFT studies of O2 activation by iron and nickel bi-metallic sites

P10
Olga Dvorackova,
University of South Bohemia
Reactivity of platinum anticancer complexes - theoretical results of QC computations

P11
Reinhold Fink,
University of Tübingen
Molecular agregate structures determined by repulsive rather than attractive interactions

P12
Marta Gałyńska,
Nicolaus Copernicus University
Does the localized state exists? Multiconfigurational study of the charge transfer process in a simple diamine cation.

P13
Leon Gerndt,
Humboldt Universitaet zu Berlin
Quantum chemical study of an Ir-catalyzed dehydrogenation reaction

P14
Tomasz Gryber,
Institute of Physical Chemistry PAS
Simulation and analysis of the relaxation dynamics of a photochromic furylfulgide

P15
Habiba Haddad, Bensiradj Nour El Houda
DFT studies of potassium clusters in Algerian groundwater

P16
Marlisa Hagemann,
University of Southern Denmark
Comparison of oxidative damage and protection mechanisms for two members of the AA9 LPMO family

P17
Hao Jiang,
Lund University
Protonation of Homocitrate and the E1 State of Fe-Nitrogenase Studied by QM/MM Calculations

P18
Michał Kochman,
Institute of Physical Chemistry PAS
Simulating the photophysics of DMABN: what have we learned, and where do we go from here?

P19
Oceane Mangel,
Université Grenoble Alpes
Study of the Streptomyces tyrosinase reaction mechanism: a dynamic QM/MM approach

P20
Zachary Mathe
Investigating Metal-Metal Bonding in Heterometallic Iron-Sulfur Clusters with XAS and DFT

P21
Markella Aliki Mermigki,
Max Planck Institut für Kohlenforschung
Evaluation of competing models for the high-spin forms of the S2 state of the oxygen-evolving complex

P22
Dariusz G. Piekarski,
Institute of Physical Chemistry PAS
Theoretical insights into tuning the enantioselectivity for anion-binding organocatalysis

P23
James Pogrebetsky,
Institute of Physical Chemistry PAS
MP2-based correction scheme to approach the limit of a complete pair natural orbitals space in DLPNO-CCSD(T) calculations

P24
Ashish Tamhankar,
Max Planck Institute for Chemical Energy Conversion
Second sphere residue effects on K-edge X-ray absorption spectroscopy and reactivity in Lytic Polysaccharide Monooxygenases

P25

Zuzanna Wojdyla,
J. Heyrovský Institute of Physical Chemistry

Role of Three-Component Thermodynamics in Reactivity and Mechanism of Radical Transfer Reactions

P26

Małgorzata Zienkiewicz-Machnik,
Institute of Physical Chemistry PAS

Experiment and theory cooperation in studies of structurally similar biomimetic Cu(II) and Co(II) cationic-anionic N-scorpionate liganda complexes with different catalytic activity

P27

Nafila Zouaghi

Theoretical (DFT) and experimental studies, reactivity descriptors calculated of Natural compounds

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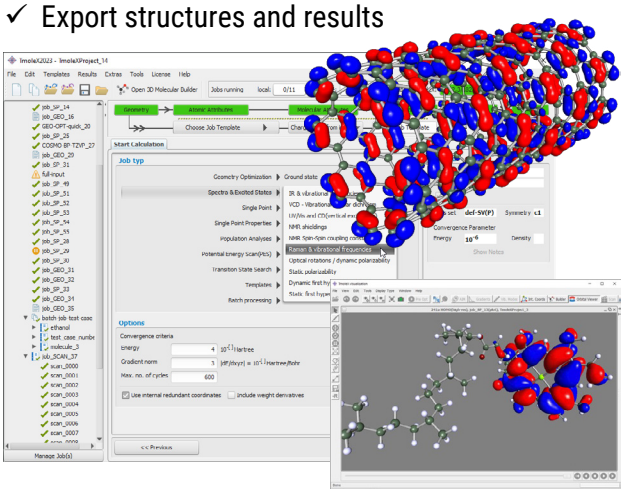

[1]*TmoleX is a product of Dassault Systèmes and is included free of charge in the TURBOMOLE program package for academic and non-profit customers.*

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