



**JERZY HABER INSTITUTE OF CATALYSIS  
AND SURFACE CHEMISTRY  
POLISH ACADEMY OF SCIENCES**



## **RESEARCH REPORT**

**General information  
for years 2014-2016**



## **Contents**

Introduction	<b>3</b>
Statistics	<b>6</b>
Research groups and laboratories	<b>7</b>
Research themes and projects	<b>9</b>
Scientific output of the Institute	<b>16</b>
Printed scientific publications	<b>16</b>
Presentations at conferences	<b>42</b>
Conferences and scientific events organized by the Institute	<b>63</b>

# **Introduction**

## **Research**

The Jerzy Haber Institute of Catalysis and Surface Chemistry of the Polish Academy of Sciences is the only scientific institution in Poland and one of very few in the world devoted entirely to research in catalysis and the chemistry of interfaces. The Institute pursues interdisciplinary studies of phenomena occurring at gas-solid, gas-liquid and liquid-solid interfaces, combining significant aspects of chemistry, physics, chemical technology, material engineering, and more recently of biology and medicine. The fundamental theoretical and experimental studies carried out in the Institute are combined with applied research so that the results obtained can be used directly to improve materials, methods or technological processes.

The Institute employs over 120 people, of whom almost 90 are research staff. Approximately 38 PhD students are also involved in research.

The research activity of the Institute focuses on four fundamental areas:

1. Catalytic materials and processes for sustainable development
2. Physics and chemistry of surfaces and nanostructures – experiment and theory
3. Nanostructures of soft matter
4. Physics and chemistry in cultural heritage protection

In the area of catalysis, much effort is put into developing new, ‘intelligent’ materials with well-defined structure and properties, tuneable to the requirements of particular catalytic reactions. ‘Green chemistry’ reactions, optimised to improve energy-efficiency and to eliminate or limit side-products are just some of the major points of interest. Enzymes and their synthetic mimics are our dynamically developing research field. With the use of theoretical and experimental methods, we try to elucidate at the molecular level catalytic mechanisms of the studied systems and develop useful biocatalysts.

In the field of surface chemistry of dispersed systems, investigations are focused on the description of adsorption phenomena and understanding the mechanism of formation and stability of foams, nano and colloid particles and their interactions, processes of microencapsulation and the biocompatibility of materials. Experimental studies are carried out in close synergy with theoretical investigations. Quantum chemical methods are used as tools to identify and characterize various electronic and structural factors influencing the selectivity and direction of chemical processes in order to explain molecular mechanism of heterogeneous and enzymatic catalytic reactions. Further, solid state physics modelling methods, as well as molecular mechanics and Monte-Carlo simulation techniques are applied.

The investigation outcomes are turned into applications encompassing catalytic materials and processes for pollutant removal to protect the environment, the manufacturing of innovative biomedical materials and the improvement of materials and methods for cultural heritage conservation. By way of example, fundamental research elucidating mechanisms of adsorption of proteins on interfaces has a considerable application potential in the processes of protein separation and purification, effective immunological tests and enzymatic reactions in bioreactors.

The institute is equipped with state-of-the-art research facilities, in many cases unique on the national scale. The equipment of joint inter-institute laboratories is also used.

In the years 2014-2016, our organizational structure consisted of 13 research groups and 2 laboratories:

#### Research groups

1. Adsorption
2. Cultural Heritage Research
3. Theoretical and Experimental Biocatalysis
4. Quantum Chemistry – Research on Catalysts and Catalytic Reactions
5. Functionalized Molecular Sieves
6. Acid-Base Catalysis (in 2016 included in the Quantum Chemistry group)
7. Catalysis in the Protection of Natural Environment
8. Colloids
9. Layered Minerals, Mesoporous Oxides, Nanostructures
10. Nanostructures of Soft Matter
11. Surface Nanostructures
12. Catalytic Processes for Clean Energy
13. Dispersed Systems

#### Laboratories:

1. XRD and Thermoanalysis Laboratory
2. Laboratory of Nanostructures and Surfaces

### **Education**

Doctoral programmes at the third-cycle level are established within three frameworks:

The International Postgraduate School, organised in collaboration with the Faculty of Chemistry, Rzeszów University of Technology.

The Interdisciplinary Doctoral Programme ‘Advanced Materials for Modern Technologies and Future Energetics’ coordinated by the Faculty of Physics and Applied Computer Science, AGH University of Science and Technology and the Institute of Nuclear Physics, Polish Academy of Sciences.

The Interdisciplinary Doctoral Programme (MOL-MED), ‘Molecular Sciences for Medicine’, which runs in cooperation with the Institute of Pharmacology of the Polish Academy of Sciences, the Faculty of Chemistry of the Jagiellonian University and the Faculty of Medicine, Collegium Medicum of the Jagiellonian University.

Number of accomplished PhD studies and PhD degrees granted in the period 2014-2016 are provided in the Statistics section below.

In the framework of cooperation with high schools, over the years 2014-2016 19 students have developed at the Institute their Master and Bachelor theses in the field of chemistry and environmental protection.

## **National and international cooperation**

The Institute has a long-standing tradition of animating and coordinating research in the field of catalysis and surface science in Poland. For almost fifty years, the Institute has organised the annual National Catalytic Colloquium, a key event for the research community in the field.

The Institute intensifies the use of its research structure by organizing joint laboratories with a number of research centres: the Centre for Surface and Nanostructure Research, the Interinstitute Laboratory of Enzymatic Catalysis and Biotechnology, the Laboratory of Electrochemistry and Surface Chemistry, Interdisciplinary Centre of Physical, Chemical and Medical Sciences, the National Laboratory for Surface Studies and SPINLAB – the National Centre of Magnetic Nanostructures for Applications in Spin Electronics.

We support the development of interdisciplinary research participating in several consortia and clusters as the Polish Technology Platform of Sustainable Chemistry, the National Consortium ‘Polish Synchrotron’, the Cluster Life Science, the Consortium ‘Catalysis in the environmental protection’ and the Consortium ‘Nanotech’, the Consortium for participation of Poland in European Research Infrastructure for Heritage Science.

In July 2012, the Institute was granted prestigious status of the National Leading Research Centre KNOW in physical sciences for 2012-2017 in the framework of the Marian Smoluchowski Krakow Research Consortium ‘Matter – energy – future’. The Consortium is formed by Faculty of Chemistry, Jagiellonian University; Faculty of Physics, Astronomy and Applied Computer Science, Jagiellonian University; Faculty of Physics and Applied Computer Science, AGH University of Science and Technology; the Jerzy Haber Institute of Catalysis and Surface Chemistry, Polish Academy of Sciences and the Henryk Niewodniczański Institute of Nuclear Physics, Polish Academy of Sciences.

The Institute is involved in extensive international cooperation. These activities include numerous bilateral international collaboration schemes, research projects of the successive Framework Programmes of the European Commission, as well as of the Operational Programmes: Innovative Economy and Human Capital, co-financed by the European Commission.

The Institute actively participates in the actions of the COST Initiative (in total 4). Between 2012 and 2016, we have coordinated COST Action CM1101 ‘Colloidal Aspects of Nanoscience for Innovative Processes and Materials’ with the participation of 70 research organisations from 36 countries.

## **Popularising research**

It is our firm belief that making scientific research easily understandable to society is of immense importance for gaining public support for investment in the field of science, both by state and private institutions. Therefore, every year, the Institute organizes Open-Door Days, during which visitors may listen to popular science lectures, participate in spectacular laboratory presentations and attend poster sessions depicting the Institute’s research. The Open-Door Days are aimed especially at young people from junior and senior high schools. They are very popular among local schools – every year the Institute receives approximately 1,000 visitors.

The Institute participates in the annual Krakow Science Festival in the city’s Main Market Square.

## Statistics 2014-2016

	2014	2015	2016	$\Sigma$
Publications				
monographs	1	1	2	2
chapters in monographs	5	7	4	16
articles in journals evaluated in Thomson Reuters Journal Citation Reports	105	94	110	309
articles in other journals and books	18	23	21	62
Patents	1	1	4	6
Patent applications	2	9	2	13
Domestic research projects	$\Sigma$	44	41	35
granted in a given year		5	5	6
International research projects	$\Sigma$	13	12	7
granted in a given year		1		1
Participation in conferences				
invited lectures	22	20	21	63
orals	82	121	73	276
posters	229	243	208	680
Participated conferences (oral presentations)	62	69	52	183
Conferences &	5	8	5	18
Popular scientific events organized by the Institute	2	2	2	6
Scientific titles and degrees granted				
professor	1	1		2
DSc (habilitation) by ICSC	1	1	2	4
in other institutions		1	1	2
PhD (doctorate) by ICSC	7	18	6	31
in other institutions	2	1		3
PhD students	48	35	31	

## **RESEARCH GROUPS AND LABORATORIES**

*Heads of the research groups in italics*

*Staff members and PhD students as on December 31<sup>st</sup>, 2016*

### **Adsorption**

*Professor Tomasz Pańczyk DSc*

Associate Professor Wojciech Płaziński DSc, Agnieszka Brzyska PhD, Paweł Wolski MSc, Łukasz Kończak MSc, Barbara Jachimska DSc

PhD students: Sylwia Świątek, Karolina Tokarczyk, Karolina Gawęda, Karina Pańczyk

### **Cultural Heritage Research**

*Professor Roman Kozłowski DSc*

Marcin Strojecki PhD, Leszek Krzemień PhD, Arkadiusz Kupczak PhD, (Michał Łukomski DSc), (Łukasz Bratasz DSc)

Agata Mleczkowska - PhD student

### **Theoretical and Experimental Biocatalysis**

*Associate Professor Tomasz Borowski DSc*

Associate Professor Maciej Szaleniec DSc, Ewa Niedziałkowska PhD, Przemysław Porębski PhD, Maciej Guzik PhD, Mateusz Tataruch PhD, Anna Miłaczewska PhD, Agnieszka Rugor PhD, (Professor Ewa Broćławik DSc)

PhD students: Ewa Wierus, Beata Mrugała, Anna Kluza, Zuzanna Wojdyła, Wojciech Snoch

### **Quantum Chemistry - Research on Catalysts and Catalytic Reactions**

*Professor Małgorzata Witko DSc, Member of Polish Academy of Sciences*

Associate Professor Renata Tokarz-Sobieraj DSc, Robert Gryboś PhD, Anna Micek-Ilnicka DSc, Urszula Filek PhD

PhD students: Agnieszka Drzwińska-Matuszek, Aleksandra Kirpsza, Natalia Ogrodowicz

### **Functionalized Molecular Sieves**

*Professor Ewa Broćławik DSc, Member of Polish Academy of Arts and Sciences*

Professor Bogdan Sulikowski DSc, (Professor Mirosław Derewiński DSc), Ewa Włoch PhD, Jerzy Podobiński MSc, Mariusz Gackowski PhD

PhD students: Krystyna Durczyk, Adam Stępniewski

### **Catalysis in the Protection of Natural Environment**

*Dorota Rutkowska -Żbik DSc*

Małgorzata Ruggiero-Mikołajczyk PhD, Katarzyna Samson PhD, Michał Śliwa PhD, Wojciech Rojek MSc

PhD students: Agnieszka Kornas, Agata Żelazny, Joanna Miąsik

### **Colloids**

*Professor Zbigniew Adamczyk DSc, Member of Polish Academy of Arts and Sciences*

Associate Professor Paweł Weroński DSc, Jakub Barbasz DSc, (Anna Bratek-Skicki PhD), Aneta Michna PhD, Małgorzata Nattich-Rak PhD, Lilianna Szyk-Warszyńska PhD, Monika Wasilewska PhD, Magdalena Oćwieja PhD, Katarzyna Kusak Eng, Elżbieta Porębska, Maria Morga PhD, Paulina Żeliszewska PhD, (Piotr Batys PhD), Marta Sadowska MSc, Elżbieta Porębska PhD

PhD students: Julia Maciejewska-Prończuk, Dawid Lupa

## **XRD and Thermoanalysis Laboratory**

*Professor Wiesław Łasocha DSc*

(Dariusz Mucha PhD)

Barbara Bożek - PhD student

## **Layered Minerals, Mesoporous Oxides, Nanostructures**

*Professor Ewa Serwicka-Bahranowska DSc*

Elżbieta Bielańska PhD, Roman Dula PhD, Dorota Duraczyńska PhD, Robert Karcz PhD, Alicja Michalik-Zym PhD, Katarzyna Pamin PhD, Jan Połtowicz PhD, Małgorzata Zimowska PhD, Daria Napruszewska MSc, Joanna Kryściak-Czerwenka PhD

Joanna Piotrowska - PhD student

## **Nanostructures of Soft Matter**

*Professor Piotr Warszyński DSc*

Ewelina Jarek PhD, Marta Kolasińska-Sojka PhD, Krzysztof Szczepanowicz PhD, Marzena Noworyta Eng, Professor Paweł Nowak DSc, Grzegorz Mordarski PhD, Michał Mosiałek DSc, Magdalena Kowacz PhD

PhD students: Karolina Podgórska, Marta Łapczyńska, Magdalena Włodek, Aneta Kędra, Zofia Krasińska, Anna Kida

## **Surface Nanostructures**

*Professor Józef Korecki DSc*

Jacek Gurgul PhD, Ewa Madej PhD, Robert Socha PhD, Associate Professor Nika Spiridis DSc, Dorota Wilgocka-Ślęzak PhD, Kinga Freindl PhD, Piotr Mazalski PhD

PhD students: Joanna Wojs, Natalia Kwiatek

## **Catalytic Processes for Clean Energy**

*Professor Alicja Drelinkiewicz DSc*

Monika Góral-Kurbiel PhD, Robert Kosydar PhD, Erwin Lalik PhD, Aleksandra Pacuła PhD

PhD students: Michał Kołodziej, Tomasz Szumełda

## **Dispersed Systems**

*Professor Kazimierz Małysa DSc*

Marcel Krzan PhD, Jan Zawała DSc, Anna Niecikowska PhD

Agata Wiertel - PhD student

## **RESEARCH THEMES AND PROJECTS**

- **Leading National Research Centre** as member of the Marian Smoluchowski Krakow Research Consortium "Matter-Energy-Future"

### **STATUTORY RESEARCH**

**2014**

#### **Catalytic Materials and Processes for Sustainable Development**

- Nanomaterials Based on Layered Minerals
- Catalytic Processes with Participation of Bio-reagents
- Studies on the Transformation of Furfuryl Alcohol towards Bio-components for Fuels and Plastics
- New Peroxo-compounds of Mo(VI), W(VI) and V(V). Synthesis, Structural Studies and Applications in Oxidation Processes
- Photocatalytic Degradation Processes of Organic Pollutants in Water with the Simultaneous Action of Oxidant – Degradation Products Analysis
- Materials with Variable Porous Structures: Synthesis, Physicochemical and Catalytic Properties; Spectroscopic and Quantum-chemical Studies
- New Cathode Materials for Solid Oxide Fuel Cells

#### **Physical Chemistry of Surfaces and Nanostructures – Experiment and Theory**

- Theoretical Calculations of Catalytic Activity of Oxide Catalysts, with Special Consideration Namely Heteropolyacids
- Structural, Electron Properties and Dynamics of Surface and Nanostructures Studied with Microscopic and Spectroscopic Techniques Radiation in the Ultra High Vacuum Conditions
- Alcohol Conversion with Acidic Catalysts as a Method for Acidity Determination
- Reaction Mechanisms for Enzymes and Biomimetic Systems – Computational Studies

#### **Soft Matter Nanostructures**

- Topology and Electrokinetic Properties of Protein Monolayers on the Solid Substrate/electrolyte Interfaces. Determining Fibrinogen Conformations Using the Polymeric Micro-particle Adsorption Method
- Functional Polyelectrolyte Multilayers Films
- Influence of the Liquid Film Size and Surface Electrical Charge on Kinetics of the Three Phase Contact Formation at Solid Surfaces of Different Hydrophobicity
- Molecular Modeling and Prediction of Properties of Selected Systems with Potential Biomedical Importance

#### **Physical Chemistry in the Protection of Cultural Heritage**

- Model Development for the Particulate Matter Deposition in the Interiors of Historical Buildings

## **2015**

### **Catalytic Materials and Processes for Sustainable Development**

- Heteropolyacid-oxide Systems; their Physicochemical Properties and Catalytic Conversion of Isopropanol
- Catalytic Processes with Participation of Bio-reagents
- New Peroxo-compounds of Mo(VI), W(VI) and V(V). Synthesis, Structural Studies and Applications in Oxidation Processes
- Studies on the Transformation of Furfuryl Alcohol towards Bio-components for Fuels and Plastics
- Hydrogenation of Acetol in the Presence of Metallic Catalysts Supported on Mesoporous Silicas
- Heteropoly Compounds as Catalysts for Oxidation of Cyclohexanone to  $\epsilon$ -Caprolactone with Molecular Oxygen
- Selective Hydrogenation of Benzene on Metal Catalysts
- Photocatalytic Activity of Layered Minerals Pillared with Transition Metal Oxides
- The Mechanism of Oxygen Reduction Reaction on Selected Cathode Materials Devoted to the High-temperature Fuel Cells

### **Physical Chemistry of Surfaces and Nanostructures – Experiment and Theory**

- Enzymatic and Biomimetic Reactions Mechanisms – Theoretical Approach
- Materials with Variable Porous Structures: Synthesis, Physicochemical and Catalytic Properties, Spectroscopic and Quantum-chemical Studies
- Structural, Electron and Dynamics Properties of Surface and Nanostructures Studied with Microscopic and Spectroscopic Techniques in the Ultra High Vacuum Conditions
- Studies of the Influence of Microscopic and Physicochemical Parameters on the Ability of Control the Properties of Systems with Biomedical Importance
- Theoretical Calculations of Catalytic Activity of Heteropolyacids Salts

### **Soft Matter Nanostructures**

- Topology and Electrokinetic Properties of Protein Monolayers on the Solid Substrate/Electrolyte Interfaces. Determining Conformations of Albumin Molecules Using the Micro-particle Deposition Method
- Influence of Ionic and Non-ionic Surface active Substances on Kinetics of the Three Phase Contact Formation at Hydrophilic and Hydrophobic Solid Surfaces
- Functional Polyelectrolyte Multilayers Films

### **Physical Chemistry in the Protection of Cultural Heritage**

- Model Development for the Particulate Matter Deposition in the Interiors of Historical Buildings

## **2016**

### **Catalytic Materials and Processes for Sustainable Development**

- Catalytic processes using bio-resources
- New peroxo- and polyoxo- compounds of Mo(VI), W(VI) and V(V). Synthesis, structural studies and applications in oxidation processes

- Catalytic oxide systems for production high value added products – components of fuels and plastics
- Hydrogenation of acetol in the presence of metallic catalysts supported on micro- and mesoporous carriers
- Heteropoly compounds as catalysts for oxidation of cyclohexanone to ε-caprolactone with molecular oxygen
- Selective hydrogenation of benzene on metal catalysts
- Photocatalytic activity of layered mineral/transition metal oxide composites
- New composite cathode materials for high temperature fuel cells
- Enzymatic redox processes

### **Physical Chemistry of Surfaces and Nanostructures – Experiment and Theory**

- Physical and chemical properties of heteropolycompounds and their catalytic activity in conversion of alcohols. DFT calculations vs. experiment
- Materials with variable porous structures: synthesis, physicochemical and catalytic Properties, spectroscopic and quantum-chemical studies
- Structural, electron and dynamics properties of surface and nanostructures studied with microscopic and spectroscopic techniques in the ultra-high vacuum conditions
- Studies of the influence of microscopic and physicochemical parameters on the ability to control the properties of systems with biomedical importance

### **Soft Matter Nanostructures**

- Topology and electrokinetic properties of protein monolayers on the solid substrate/electrolyte interfaces. Determining conformations of blood serum proteins by streaming potential measurements and nanoparticle and polymeric microparticle deposition
- Determination of mechanisms of synthesis, structure, and transport parameters of supported colloidal particle multilayers
- Influence of kinetic energy on kinetics of bubble coalescence at free surface of pure liquids
- Functional multilayer polyelectrolyte films

### **Physical Chemistry in the Protection of Cultural Heritage**

- Modelling environmental conditions and energy consumption in buildings preserving cultural heritage assets

## **RESEARCH PROJECTS**

### **Research Projects of the Ministry of Science and Higher Education**

- N N204 205240 [2011-2014] Studies of Structure and Properties of a Magnetically Triggered Molecular Nanocontainer
- N N204 133640 [2011-2014] Influence of Micro- and Nano-bubbles at Hydrophobic Surfaces on Kinetic and Mechanism of the Three Phase Contact Formation in Milliseconds Timescale
- N N204 439640 [2011-2014] Quantum-chemical Studies on the Mechanism of Transmetallation Reaction of Porphyrin and its Selected Derivatives
- N N204 439040 [2011-2014] The New Multi-layered Systems with Controlled Architecture and Functionality
- N N209 757340 [2011-2014] Application of Membrane Emulsification for Formation of Nano- and Microcapsules' Cores

### **"Sonata Bis" Research Projects of the National Science Centre**

- ST4 [2013-2017] Computer Aided Design and Prediction of Properties of Drug Delivery Systems Based on the Structure of Carbon Nanotubes
- NZ1 [2015-2020] 2-Oxoglutarate Dependent Oxygenases in the Biosynthesis of Pharmacologically Active Alkaloids - Structure, Catalytic Mechanisms and Rational Redesign
- ST4 [2016-2020] Molecular mechanics force field for structure, dynamics and conformation of carbohydrates involving furanoses

### **"Sonata" Research Projects of the National Science Centre**

- HS2 [2011-2014] Impact of Heating Historic Churches on Transfer and Deposition of Dust
- ST5 [2011-2016] New Pd-Pt/Hybrid Nanocomposite Catalysts for Oxygen Reduction in Polymer Electrolyte Membrane Fuel Cell
- ST5 [2011-2014] Functionalization of the Polymer Films as a Tool for Attainment of the Novel Materials of Broad Utility Spectrum
- ST4 [2012-2015] Conformational Changes of the Pyranose Rings: Computer Simulations
- ST5 [2012-2017] Targeted Drug Delivery Systems - Synthesis and Functionalization of Nanocarriers
- ST4 [2013-2017] The Mechanism of Regioselective Oxidation of Cholesterol Derivatives by a Novel Molybdenum Enzyme, Steroid 25-OH Dehydrogenase from *Stereolibacterium denitrificans*
- ST4 [2013-2017] Mechanism and Kinetics of Bubble Coalescence at Undisturbed and Vibrating, with Controlled Frequency and Amplitude, Liquid/gas Interfaces
- ST4 [2015-2018] New Protein Bilayer System Based on Antigen-Antibody Interactions – *In situ* Physicochemical Characteristics

### **"Opus" Research Projects of the National Science Centre**

- HS2 [2011-2014] Mechanism of Damage of Panel Paintings Taking into Account Growth Ring Structure of Wood and Real World Climate Fluctuations
- ST8 [2011-2014] New Development in Technology of Stable and Biodegradable Foam Generation - for Industrial and Biomedical Applications
- ST5 [2012-2015] Influence of Glycerol as Non-Toxic and Biodegradable Solvent on the Mechanism of Phenol Oxidation
- ST4 [2012-2014] Properties of Chromium(VI), Molybdenum(VI) and Tungsten(VI) Monomeric Oxo Species on Amorphous Silica and Al-Modified Silica from Periodic DFT Simulations
- ST4 [2012-2015] Physicochemical and Catalytic Properties of Heteropolyacids Modified with Copper Ions. Theoretical Calculations vs. Experiment
- ST4 [2012-2015] Mechanism of Ionic Surfactant - Polyelectrolyte Interactions in the Process of Formation of New Generation of Nanocarrier
- NZ1 [2012-2016] Structure and Function of Acireductone Dioxygenases – Experimental and Computational Studies
- ST4 [2013-2016] The Surface Chemistry Studies of the Hybrid Catalysts as the Method for the Explanation of Their Catalytic Properties in the High Pressure Dimethyl Ether Synthesis from the H<sub>2</sub>/CO<sub>2</sub> Mixture
- ST5 [2013-2016] Novel Layered Porous Materials Based on Zeolite Nanoclusters for the Liquid-Phase Catalytic Processes
- ST5 [2013-2016] Design, Synthesis, and Physicochemical Characterization of Ruthenium Catalysts and Their Application in Hydrogenation od Prochiral Ketones

- ST4 [2013-2016] Dynamics of Oscillations in the Palladium/Hydrogen System
- ST4 [2013-2016] Adsorption Mechanisms of Anisotropic Proteins under Controlled Transport Conditions
- ST4 [2013-2016] Structure and Properties of Protein Layers: from Biomolecules to a Functional Layer (A Combined Experimental and Simulation Study)
- ST5 [2014-2017] Synthesis and Physicochemical Characterization of the Electrocatalysts Containing Non-noble (Fe, Mn) and Noble (Pd) Metals Deposited on Porous N-Doped Carbon Materials with Different Morphologies and Examination them in Oxygen Reduction Reaction
- ST5 [2014-2017] Innovative Total Oxidation Catalysts Derived from Organosmectites Intercalated with Reverse Micelles Containing Oxide/hydroxide Nanostructures
- NZ1 [2015-2017] 2-Oxoglutarate Dependent Oxygenases Catalyzing Atypical Oxidative Transformations - Structural and Mechanistic Studies
- ST5 [2016-2019] Theranostic nanocarriers for MRI imaging
- ST5 [2016-2019] A new generation of hierarchical Y and omega zeolite catalysts: advanced IR and NMR studies and molecular modeling
- ST5 [2016-2019] Nanoparticle monolayers of controlled heterogeneity and structure as efficient antifouling substrates

#### **"Preludium" Research Projects of the National Science Centre**

- ST5 [2012-2014] Synthesis of biocompatible nanocarriers for selected neuroprotective agents
- ST4 [2013-2015] Improving the Method of Detection of Hydrogen Peroxide by Modifying Films Containing Prussian Blue Nanoparticles by Conductive Polymers and Reduced Graphene Oxide Sheets
- ST5 [2013-2015] Multilayer Polymer Films Containing Nanoparticles and Graphene as a Functional Coatings and Membranes
- ST5 [2013-2015] Electrokinetic Characteristics of Interaction between Recombinant HSA Monolayers and Ionic Ligands
- ST4 [2013-2015] Determining Mechanisms of Fibrinogen Adsorption on Colloids Particles
- ST4 [2014-2016] Electronic Coupling of Nitric Oxide with Cobalt Centers in Various Coordination Environments: Impact of Electron Density Flow on Ligand Activation
- ST4 [2014-2016] Mechanism of Irreversible Nanoparticles Adsorption on Colloids Particles
- ST4 [2016-2017] Polyelectrolyte-lipids films with incorporation hydrophobic nanoparticles

#### **"Harmonia" Research Projects of the National Science Centre**

- ST4 [2013-2015] Visualizing the Local Reaction Kinetics: From the Mesoscopic to the Nanoscale

#### **"Fuga" Research Projects of the National Science Centre**

- ST3 [2015-2018] High resolution analysis of the spatial properties of structured magnetic nanostructures
- ST4 [2015-2018] Effect of electromagnetic radiation in the infrared range on protein-surface interactions

#### **"Iuventus Plus" Programme Projects of the Ministry of Science and Higher Education**

- IP2011 0353 71 [2012-2014] A New Method of Silver Sol Synthesis and Mechanism of Colloidal Particles Interaction with Heterogeneous Surfaces Determined by Electrokinetic Phenomena and AFM, Fluorescent Microscopy and QCM-D Techniques

- IP2012 006372 [2013-2015] The Advanced Theoretical Study on the Mutarotation Reaction of D-Glucopyranose
- IP2012 058972 [2013-2015] Magnetic Responsive Drug Delivery Systems with the Controlled Release Properties
- [2014-2016] Theoretical Modeling of Influence of Liquid/Gas Interface Fluidity Variations on Kinetics of Bubble Collision with Liquid/Gas and Liquid/Solid Interfaces
- [2016-2019] Determination of the influence of surface properties of silver nanoparticles on their cytotoxic activity towards the human cells of immune system and the cells of connective tissues

#### **"Pomost" Programme Research Projects of the Polish Foundation for Science**

- FNP 2011-3/7 [2011-2014] Selective Hydrogenolysis of Glycerol to Glycols via Acetol on Heterogeneous Metal/Metal Oxides Based Catalysts

#### **Strategic Research Projects of the National Centre for Research and Development**

- NCBiR SP/J/7/170071/12 [2012-2015] NUCLEAR Catalysts for Recombination of Hydrogen and Oxygen in Nuclear Reactors. Catalysts Activity as a Crucial Parameter Determining Safety of Recombiners Performance

#### **Applied Research Programme Projects of the National Centre for Research and Development**

- NCBiR PBS2/A9/24/2013 [2013-2017] HERIVERDE Energy Efficiency of Museum and Library Institutions

#### **"Leader" Programme Research Projects of the National Centre for Research and Development**

- NCBiR LIDER/33/147/L-3/11/NCBR/2012 [2012-2016] Regioselective Oxidation of Cholesterol Derivatives with a Novel Molybdoenzyme – 25-OH Cholesterol Dehydrogenase

#### **EC 7<sup>th</sup> Framework Programme Projects**

- EC FP7-NMP-2012-CSA-6 [2012-2015] NanoIES Nanotechnology Education for Industry and Society (CSA)
- EC 7<sup>th</sup> 310420 [2013-2015] HYPERCONNECT Functional Joining of Dissimilar Materials Using Directed Self-Assembly of Nanoparticles by Capillary-Bridging (CP)

#### **EU COST Actions**

- EU COST Action CM1101 [2012-2016] Colloidal Aspects of Nanoscience for Innovative Processes and Materials
- EC COST CM 1305 [2012-2016] ECOSTBio Explicit Control Over Spin-states in Technology and Biochemistry
- EC COST CM1203 [2012-2016] PoCheMoN Polyoxometalate Chemistry for Molecular Nanoscience
- EC COST EU COST Action MP1106 [2012-2016] SGI Smart and Green Interfaces - from Single Bubbles and Drops to Industrial, Environmental and Biomedical Applications

#### **Projects of the Polish-Norwegian Research Programme**

- [2013-2016] NANONEUCAR Nanoparticulate Delivery Systems for Therapies Against Neurodegenerative Diseases

- [2013-2015] FUNClay Synthesis and Functionality of Innovative Porous Clay Hybrid Nanostructures
- [2014-2016] InlinePV In-line Processing of n+/p and p/p+ Junction System for Cheap Photovoltaic Module Production

### **Projects of EU Structural Funds Programmes**

- PO KL 4.1.1 [2009-2015] ISD Advanced Materials for the New Technologies and Energy of the Future
- PO IG 1.3.1. [2009-2014] BIOTRANSFORMACJE Biotransformations Useful in Pharmaceutical and Cosmetics Industry
- POIG 1.1.2. [2009-2014] FUNANO Functional Nano- and Microparticles, Synthesis and Applications in Innovative Materials and Technologies
- PO KL 4.1.1 [2010-2015] ISD MOLMED Molecular Sciences for Medicine

### **Other International Projects**

- Intergovernmental Polish-Slovak Project [2013-2015] Organo-Clays as Intermediates for the Synthesis of Functional Hybrid Materials
- Intergovernmental Polish-Slovak Project [2016-2018] Immobilization of metal nanoparticles on organo-modified layered silicates
- SCIEX Project [2014] Advanced Computer Simulations of Hyaluronan Conformational Properties

### **Projects of the Consortium "Coal Fuel Cells" under auspices of the Ministry of Economy+**

- [2012-2014] Molten Carbonate Electrolyte Direct Carbon Fuel Cell (DC-MCFC)

# **SCIENTIFIC OUTPUT OF THE INSTITUTE**

## **Printed scientific publications**

**2014**

### **Monographs**

1. M.Oćwieja "Kinetyka tworzenia oraz stabilność monowarstw nanocząstek srebra. Badania podstawowe w dobie dynamicznego rozwoju nanotechnologii" (T.Czarnik, ed.), Wydawnictwo Bezkresy Wiedzy, Saarbrücken 2014, pp.248 [ISBN 978-3-639-89158-4]

### **Chapters in monographs**

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2. "16<sup>th</sup> International Conference on Theoretical Aspec5ts of Catalysis, Zakopane, Poland, 19<sup>th</sup>-23<sup>rd</sup> June, 1016", (D.Rutkowska-Żbik, ed.), IKiFP PAN Kraków, 2016, pp.104 [ISBN 978-83-60514-25-2]

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1. Z.Adamczyk "Nanoparticle and protein adsorption guest for a universal mechanism", Conf. Nanotechnology: Research and Development, Vilnius 2014
2. Z.Adamczyk "Protein Adsorption - Mythology and (or) Science", 5<sup>th</sup> US-Poland Workshop: Thermodynamics of Complex Fluids and Interfaces, Warszawa 2014
3. Z.Adamczyk, M.Morga, A.Michna "Adsorption Mechanisms of Polyelectrolytes and Proteins", 20<sup>th</sup> Int. Symp. on Surfactants in Solution SIS 2014, Coimbra 2014
4. T.Borowski "Spin states and reaction mechanisms of mononuclear non-heme metalloenzymes - computational studies", COST Action CM1305 First Scientific Workshop, Girona 2014
5. E.Brocławik, M.Radoń, T.Borowski, A.Stępniewski "Spin- and electron density redistribution upon binding of noninnocent ligand by iron and related TM sites in enzymatic environment", Conf. From Computational Biophysics to Systems Biology CBSB14, Gdańsk 2014
6. E.Brocławik, A.Stępniewski, K.Góra-Marek, M.Radoń "Donor modifiers of Co(II) active sites: explicit spin and charge transfer channels for NO - NH<sub>3</sub> co-adsorption in zeolites", Conf. Modelling and Design of Molecular Materials, Kudowa Zdrój 2014
7. A.Drelinkiewicz, E.Lalik, R.Kosydar, W.Rojek, J.Gurgul, T.Szumelda, M.Kołodziej, R.Tokarz-Sobieraj "Kataliza – bezpieczeństwo reaktorów nuklearnych", Konf. Struktura a Reaktywność Układów Metal/Nośnik, Falenty 2014
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12. T.Korona, H.Dodziuk, A.Hesselmann, D.Rutkowska-Żbik "Endohedral complexes of fullerenes and other large complexes - what can we get from contemporary ab initio methods?", Polish-Taiwanese Conf. 'From Molecular Modeling to Nano-and Biotechnology', Opole 2014
13. W.Łasocha, K.Luberda Durnaś "New hybrid organic-inorganic materials, Synthesis, structure, applications", E-MRS, 2014 Fall Meeting Warszawa 2014
14. W.Łasocha, A.Szymańska, M.Oszajca, G.Appleby, K.Pamin, J.Poltowicz "Polymolybdates and Peroxomolybdates: Candidates for Catalysts in Industry", 23<sup>th</sup> Congr. of Int. Union of Crystallography, Montreal 2014
15. M.Mosiałek, M.Dudek, P.Nowak, R.P.Socha "Silver migration caused by polarization at the Ag|Al<sub>0.04</sub>Sc<sub>0.06</sub>Zr<sub>0.9</sub>O<sub>1.95</sub> interface" Int. Symp. on Clean Energy from Ethanol ISCEE 2014, Rzeszów2014

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2. P.Batys, M.Nosek, P.Weroński "Application of Monte Carlo method for adsorption process simulation", CCP5 Summer School 2014 Methods in Molecular Simulations, Manchester 2014
3. P.Batys, P.Weroński "Transport properties of layer-by-layer assemblies of spherical particles at solid/liquid interface", IX<sup>th</sup> Summer School for Graduate Students: Interfacial Phenomena in Theory and Practice, Sudomie 2014
4. M.Bobruk, M.Kopeć, T.Chmielewski, P.Nowak "Stoichiometry of copper sulfides and the electrosorption of xanthates", Mineral Engineering Conf. MEC 2014, Istebsa 2014
5. T.Borowski "Quantum mechanics/molecular mechanics (QM/MM) methods – foundations & examples of bio-applications", 3<sup>rd</sup> Int. Conf. of Biophysics Students, Kraków 2014
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8. K.Durczyk, B.Sulikowski "Ultrastabilne formy zeolitu typu Y: otrzymywanie i właściwości fizykochemiczne", 3. Ogólnopolska Konferencja 'Pomiędzy Naukami', Zjazd Fizyków i Chemików, Chorzów 2014
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14. J.M.del Hoyo-Meléndez, M.Matosz, Ł.Bratasz "XRF analysis of metallic cultural heritage objects from the National Museum in Krakow", 3<sup>rd</sup> Int. Congr. Chemistry for Cultural Heritage CHEMCH 2014, Wien 2014
15. B.Jachimska, K.Bieda "Structure of Adsorbed Dendrimer Monolayers Investigated by Combining QCM-D and MP-SPR Techniques", Symp. of the Analytical Division of SPQ-2014, Coimbra 2014
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19. Ł.Kończak, T.Pańczyk "Molecular dynamics simulations of proton transverse relaxation times in suspension of magnetic nanoparticles", Central European School on Physical Organic Chemistry, Przesieka 2014
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27. K.Kubiak, A.Michna, Z.Adamczyk, K.Jamroży "PDADMAC Deposition studies - QCM and streaming potential measurements", IX<sup>th</sup> Summer School for Graduate Students: Interfacial Phenomena in Theory and Practice, Sudomie 2014

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35. A.Miłaczewska, T.Borowski "Insight into a reaction mechanism of acireductone dioxygenation – DFT studies for a model system", 46. Ogólnopolskie Kolokwium Katalityczne, Kraków 2014
36. A.Mleczkowska, Ł.Bratasz, R.Kozłowski, M.Strojecki "Zabrudzenia wnętrz zabytkowych kościołów – źródła pyłów, ich przenoszenie i osiadanie", 14. Konf. Analiza Chemiczna w Ochronie Zabytków, Warszawa 2014
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41. M.Oćwieja, Z.Adamczyk, B.Szaraniec, M.Kujda "Mechanizm uwalniania nanocząstek srebra w zastosowaniach praktycznych", 57. Zjazd Naukowy PTChem i SITPCh, Częstochowa 2014
42. M.Oćwieja, A.Gorczyca, E.Pociecha "Wpływ nanocząstek srebra na rozwój i funkcjonowanie wybranych mikro- i makroorganizmów", Konf. Małopolski Festiwal Innowacji, Kraków 2014
43. J.Olszówka, E.Bielawska, B.Napruszewska, A.Michalik-Zym, E.M.Serwicka "Katalityczne utlenianie cykloheksanonu do ε-kaprolaktonu przy użyciu nadlitenku wodoru w obecności katalizatorów zawierających magnez", 46. Ogólnopolskie Kolokwium Katalityczne, Kraków 2014
44. J.Olszówka, R.Karcz, B.Napruszewska, E.M.Serwicka "Catalytic oxidation of cyclohexanone to ε-caprolactone with hydrogen peroxide over hydrotalcite catalysts", 12<sup>th</sup> Chemistry Conf. for Young Scientists, Blankenberge 2014

45. A.Pajor-Świerzy, T.Kruk, P.Warszyński "The Influence of Reduced Graphene Oxide and Conductive Polymers on the Electrocatalytic Properties of the Polyelectrolyte Multilayer Films Containing Prussian Blue Nanoparticles", 28<sup>th</sup> Conf. of the European Colloid and Interface Soc. ECIS2014, Limassol 2014
46. K.Pamin "Heteropolizwiązki jako katalizatory transformacji węglowodorów", 13. Konf. Elektroanaliza w Teorii i Praktyce, Kraków 2014
47. K.Pamin, J.Połtowicz, M.Prończuk, S.Basąg, J.Maciejewska "Hydroxylation of phenol by hydrogen peroxide catalyzed by heteropoly compounds in presence of glycerol as green solvent", 3<sup>rd</sup> Int. Symp. on Air & Water Pollution Abatement Catalysis AWPAC, Kraków 2014
48. P.Panek, K.Drabczyk, R.P.Socha, P.Zięba "Wpływ tylnej warstwy typu p+ na parametry ogniw słonecznego na bazie krzemiu typu p na podstawie obliczeń wykonanych programem komputerowym PC-1D", 5<sup>th</sup> Symp. on Photovoltaics and Transparent Electronics - Development Perspectives, Świeradów-Zdrój 2014
49. G.Para, E.Jarek, J.Łuczyński, K.A.Wilk, P.Warszyński "Adsorption of ionic-nonionic surfactant mixtures at water/air interface - alkanoic acids and cleavable cationic surfactants", COST Action CM1101 WG1, WG3, WG5 & WG6 Meeting Particles at Liquid and Solid Interfaces: Fundamentals and Applications, Genoa 2014
50. G.Para, E.Jarek, J.Łuczyński, K.A.Wilk, P.Warszyński "Adsorption of ionic-nonionic surfactant mixtures at water/air interface - alkanoic acids and cleavable cationic surfactants", 20<sup>th</sup> Int. Symp. on Surfactants in Solution SIS 2014, Coimbra 2014
51. M.Piotrowski, K.Szczepanowicz, D.Jantas, W.Lasoń, P.Warszyński "Emulsion-Core and Polyelectrolyte-Shell Nanocapsules as Drug Delivery System for Undecylenic Acid", Conf. Nanocon 2014, Brno 2014
52. A.Płazińska, W.Płaziński, K.Jóźwiak "Prediction of the stereochemical effects in the ligand-receptor interactions: metadynamics simulations", Conf. Bioinformatics in Toruń BIT14, Toruń 2014
53. W.Płaziński, M.Drach "Carbohydrate ring puckering: transition path sampling analysi", 27<sup>th</sup> Int. Carbohydrate Symp., Bangalore 2014
54. A.Rugor, A.Dudzik, N.Zawada, S.Mordalski, J.Staroń, A.Bojarski, M.Szaleniec "Badania nad strukturą i aktywnością katalityczną Dehydrogenazy C25 steroidowej z Sterolibacterium Denitrificans", 46. Ogólnopolskie Kolokwium Katalityczne, Kraków 2014
55. A.Rugor, T.Janeczko, A.Dudzik, J.Staroń, A.Bojarski, M.Szaleniec "Selective modifications of sterols performed by enzymes from Sterolibacterium denitrificans", 2<sup>nd</sup> Symp. on Biotransformations for Pharmaceutical and Cosmetic Industry, Warszawa 2014
56. M.Skoczek, P.Batys, P.Weroński, E.Luchter-Wasylewska "Quantitative characterization of model prostatic membrane - molecular dynamic simulations", IX<sup>th</sup> Summer School for Graduate Students: Interfacial Phenomena in Theory and Practice, Sudomie 2014
57. R.P.Socha, A.Kędra, M.Zimowska, P.Panek, L.Szyk-Warszyńska, M.Lipiński, P.Warszyński "The morphology and surface chemistry of silicon etched with bimetallic catalysts", 30<sup>th</sup> European Conf. on Surface Science ECOSS 30, Antalya 2014
58. R.P.Socha, A.Kędra, M.Zimowska, P.Panek, L.Szyk-Warszyńska, M.Lipiński, P.Warszyński "The studies on application of the metallic and bimetallic catalysts for silicon etching", 5<sup>th</sup> Symp. on Photovoltaics and Transparent Electronics - Development Perspectives, Świeradów-Zdrój 2014
59. R.Socha, M.Ślęzak, M.Szczepanić-Ciba, N.Spiridis, D.Wilgocka-Ślęzak, T.Giela, N.Pilet, J.Raabe, J.Korecki "CO oxidation on MnO/Pt(111) studied by XPS, TPD, XAS and PEEM", 30<sup>th</sup> European Conf. on Surface Science ECOSS 30, Antalya 2014
60. A.Stępniowski, K.Góra-Marek, M.Radoń, E.Brocławik "Influence of Ammonia Co-adsorption on Spin and Electron Transfer for Co(II) Sites in Zeolites: IR Studies on NO Activation and DFT Modeling", 6<sup>th</sup> FEZA Conf. Leipzig 2014

61. M.Szaleniec, P.Dyshlovenko, L.Szyk-Warszyńska, P.Warszyński "Description of protein adsorption in terms of colloidal interactions", COST Action CM1101 WG2 & WG5 Meeting Interactions in Colloidal Systems, Berlin 2014
62. M.Szaleniec, P.Dyshlovenko, L.Szyk-Warszyńska, P.Warszyński "Can we Describe Protein Adsorption in Terms of Electrostatic Interactions?", 28<sup>th</sup> Conf. of the European Colloid and Interface Soc. ECIS2014, Limassol 2014
63. M.Szaleniec, A.Rugor, J.Heider, T.Borowski, M.Witko "Monomolybdenum enzymes hydroxylating hydrocarbons – isotope experiments and modeling of mechanism", 15<sup>th</sup> Int. Conf. on Theoretical Aspects of Catalysis ICTAC15, London 2014
64. M.Szaleniec, A.Rugor, E.Niedziałkowska, A.Dudzik, M.Tataruch, D.Knack "Biocatalytic Hydroxylation of Cholesterol and Its Derivatives", Conf. Life Science Open Space 2014, Kraków 2014
65. M.Szczepanik-Ciba, M.Ślęzak, T.Giela, D.Wilgocka-Ślęzak, N.Pilet, J.Raabe, N.Spiridis, J.Korecki "LEEM/PEEM investigation of epitaxial metal and oxide manganese nanostructures on W(110)", European Conf. on Surface Science ECOSS 30, Antalya 2014
66. K.Szczepanowicz, A.Karabasz, M.Bzowska, S.Łukasiewicz, P. Warszyński "Targeted drug delivery system based on polyelectrolyte nanocapsules", COST Action CM1101 WG3 & WG4 Meeting Synthesis of advanced nano- and bio-colloidal materials with highly active surfaces, Belgrade 2014
67. K.Szczepanowicz, S.Łukasiewicz, M.Dziedzicka-Wasylewska, P.Warszyński "Encapsulated emulsion droplets as drug carriers", Conf. Smart and Green Interfaces, Marseille 2014
68. K.Szczepanowicz, M.Piotrowski, K.Podgórska, M.Łapczyńska, T.Kruk, L.Szyk-Warszyńska, P.Warszyński "Multiwarstwy polielektrolitów w układach dostarczania leków", Semin. Projektu POIG FUNANO 2014, Krakow 2014
69. T.Szumełda, A.Drelinkiewicz, R.Kosydar, J.Gurgul, E.Bielawska "Wpływ zawartości Au w katalizatorach bimetalicznych PdAu/C otrzymywanych metodą 'odwróconej mikroemulsji' na selektywność w reakcji uwodorniania aldehydu cynamonowego", 2. Ogólnopolskie Forum Chemii Nieorganicznej, Wrocław 2014
70. M.Ślęzak, T.Giela, D.Wilgocka-Ślęzak, N.Spiridis, T.Ślęzak, A.Kozioł-Rachwał, M.Zajac, M.Stankiewicz, N.Pilet, J.Raabe, P.Warnicke, C.Quitmann, J.Korecki "Prospects of X-ray Photoemission Electron Microscopy at the first beamline of Polish synchrotron SOLARIS", 12<sup>th</sup> Int. Symp. & School on Synchrotron Radiation in Natural Science ISSRNS-12, Warszawa 2014
71. M.Śliwa, R.Grabowski, A.Żelazny, A.Kornas, K.Samson, M.Ruggiero-Mikołajczyk, J.-F.Paul, D.Rutkowska-Żbik "Influence of polymorphic ZrO<sub>2</sub> phases and the copper electronic state on the activity of Cu/ZrO<sub>2</sub> catalysts in the hydrogenation of CO<sub>2</sub> to methanol", 3<sup>rd</sup> Int. Symp. on Air & Water Pollution Abatement Catalysis AWPAC, Kraków 2014
72. S.Świątek, B.Jachimska "Charakterystyka funkcjonalnych warstw wołowej β-laktoglobuliny (LGB)", I Semin. Naukowe Zielone Idee 21. Wieku, Poznań 2014
73. M.Tataruch, M.Szaleniec, A.Bogusławska, P.Nowak, J.Bryjak, J.Heider "Application studies on synthesis of chiral alcohols by ethylbenzene dehydrogenase", 7<sup>th</sup> Int. Congr. on Biocatalysis BIOCAT 2014, Hamburg 2014
74. R.Tokarz-Sobieraj, R.Gryboś, M.Witko, A.Micek-Ilnicka, U.Filek, A.Bielawski "Generation of acidic sites in Al, Ga, In salts of molybdenum and tungsten heteropolyacids. DFT modeling and catalytic tests", 3<sup>rd</sup> Int. Symp. on Air & Water Pollution Abatement Catalysis AWPAC, Kraków 2014
75. R.Tokarz-Sobieraj, R.Gryboś, M.Witko, U.Filek, A.Micek-Ilnicka, A.Bielawski "Al, Ga, In salts of tungsten and molybdenum heteropolyacids - theory vs. experiment", 12<sup>th</sup> Panonnian Symp. on Catalysis, Trest 2014

76. T.Wilkosz, A.Wesełucha-Birczyńska, J.Dutkiewicz, E.Bielańska, J.Camra, L.Lityńska-Dobrzyńska, P.Kornelak, M.Najbar "Rola powinowactwa do tlenu i temperatur Tammanna metali w projektowaniu monolitycznych katalizatorów środowiskowych na folii ze stali kwasoodpornej, do redukcji tlenków azotu", 46. Ogólnopolskie Kolokwium Katalityczne, Kraków 2014
77. P.Wolski, T.Pańczyk "Molecular dynamics simulations of interactions of congo red with single-walled carbon nanotubes", Central European School on Physical Organic Chemistry, Przesieka 2014
78. A.Wójcik, E.Brocławik, P.E.M.Siegbahn, T.Borowski "How subtle differences in enzyme structures affect the reaction outcome? Theoretical studies on HMS and HPPD", 46. Ogólnopolskie Kolokwium Katalityczne, Kraków 2014
79. M.Zając, A.Bianco, C.J.Bocchetta, E.Busetto, P.Goryl, J.Korecki, M.Sikora, M.J.Stankiewicz, M.Ślęzak, A.I.Wawrzyniak, Ł.Żytniak "First bending magnet beamline at Solaris", 12<sup>th</sup> Int. Symp. & School on Synchrotron Radiation in Natural Science ISSRNS-12, Warszawa 2014
80. J.Zawała, D.Kosior, K.Małyśa "Influence of surface-active substance on kinetics of the bubble attachment to hydrophobic solids", XIVth Polish- Ukrainian Symp. on Theoretical and Experimental Studies of Interfacial Phenomena and Their Technological Applications & 1st NanoBioMat Conf. Nanostructured Biocompatible/Bioactive Materials, Zakopane 2014
81. J.Zawała, D.Kosior, A.Nieciowska, K.Małyśa "Surface charge and kinetics of the three-phase contact formation at hydrophobic and hydrophilic solids", 15th Int. Conf. Surface Forces, Verbilki 2014
82. A.Żelazny, K.Samson, R.Grabowski, M.Ruggiero-Mikołajczyk, M.Śliwa, D.Rutkowska-Żbik, A.Kornas, M.Lachowska "Influence of the carrier on physicochemical and catalytic properties of Cu-Ag/oxide catalysts for selective hydrogenolysis of glycerol to propylene glycol", 12<sup>th</sup> Panonian Symp. on Catalysis, Trest 2014

## 2015

### Plenary, keynote and invited lectures

1. Z.Adamczyk "Protein Adsorption - A new paradigm", 15<sup>th</sup> Int. Conf. on Nanotechnology IEEE NANO 2015, Rome 2015
2. T.Borowski, M.Quesne, A.Miłaczewska, Z.Wojdyła, A.Wójcik "Reaction mechanisms of mononuclear metalloenzymes", Conf. Modeling Interactions in Biomolecules VII, Prague 2015
3. J.Heider, M.Szaleniec "Oxygen-independent hydrocarbon hydroxylation reactions by molybdenum enzymes: ethylbenzene dehydrogenase and family", 9<sup>th</sup> Molybdenum and Tungsten Enzymes Conf., Balatonfured 2015
4. J.Korecki "Structural and electronic properties of ultrathin iron oxide films on Pt(111): from FeO to Fe<sub>2</sub>O<sub>3</sub>", COST Action CM1104 WG1+WG2 Workshop, Kraków 2015
5. J.Korecki "Spektro-mikroskopia z użyciem miękkiego promieniowania X w 'Solaris'", 43. Zjazd Fizyków Polskich, Kielce 2015
6. M.Kujda, Z.Adamczyk; "Physicochemical characteristics of albumin dimer and its monolayers", Conf. Suspensions -designing, synthesis, properties, application SUSPENS, Krakow 2015
7. P.Niemiec, R.Tokarz-Sobieraj, R.Gryboś, A.Micek-Ilnicka, U.Filek, A.Kirpsza, M.Witko "Catalytic activity of selected heteropolyacids. Theory vs. experiment", Conf. 'Multiscale phenomena in molecular matter', Krakow 2015
8. P.Nowak, M.Mosiałek, G.Nawrat "Corrosion of magnesium and its alloys - new observations and ideas"; 18. Ogólnopolskie Symp. Naukowo-Techniczne APSCS-2015 'Nowe Osiągnięcia w Badaniach i Inżynierii Korozyjnej', Poraj 2015

9. T.Pańczyk, P.Wolski, Ł.Kończak "Nanorurki węglowe jako nośniki leków. Projektowanie na podstawie modelowania molekularnego", Konf. 40 lat Chemii Teoretycznej na Uniwersytecie Marii Curie-Skłodowskiej - Rozwój i Badania, Lublin 2015
10. M.Quesne "Utilizing QM/MM techniques inthe study of enzyme catalyses reaction mechanisms", 3<sup>rd</sup> Scientific Workshop of the COST Action CM1305 "Explicit control over spin states in technology and Biochemistry", Belgrade 2015
11. M.Quesne "How can theoretical techniques inform us of the chemistry of real world catalysts", RSC Inorganic Reaction Mechanisms Discussion Group Meeting, Manchester 2015
12. D.Rutkowska-Żbik, A.Drzewiecka-Matuszek, R.Tokarz-Sobieraj, J.Korecki, B.Szafran, A.Duschl, P.Queipo "Developing Nanotechnology Curricula to Meet Industry and Society Needs", EuroNanoForum 2015, Riga 2015
13. B.Sulikowski "Zeolites, nanoclusters and related mesoporous materials: an insight from solid-state NMR spectroscopy standpoint", 20. Forum Zeolitowe, Stryszawa 2015
14. M.Szaleniec, A.Dudzik, E.Niedziałkowska, A.Rugor, M.Tataruch "Bacterial dehydrogenases from *S. denitrificans* – biocatalytic tools for modification of sterols and steroids", Workshop on Agricultural Biotechnology and Biocatalysis, Warszawa 2015
15. M.Szaleniec, A.Dudzik, E.Niedziałkowska, A.Rugor, M.Tataruch, M.Wasylewski "Steroid C25 dehydrogenase – a novel catalyst for regioselective hydroxylation of cholesterol and its derivatives", World Congr. on Beneficial Microbes: Food, Pharma, Aqua & Beverages Industry, Valencia 2015
16. M.Szaleniec, M.Witko, J.Heider "Czy modelowanie teoretyczne jest wiarygodnym narzędziem do badania reaktywności enzymów?", 42. Ogólnopolska Szkoła Chemii 'Chemia z głębą ziemi', Lubenia 2015
17. K.Szczepanowicz, G.Para, L.Szyk-Warszyńska, K.A.Wilk, P.Warszyński "Role of surfactant/polimer complex in the formation of nanocapsules", Conf. 'Smart and Green Interfaces:Fundamentals and Diagnostics (SGI-FunD), D.Exerowa Symp.', Sofia 2015
18. T.Ślęzak, A.I.Chumakov, A.Kozioł-Rachwał, R.Ruffer, N.Spiridis, M. Ślęzak, M.Zając, J.Korecki "Resolving the complex spin structures with Nuclear Resonant Scattering", 22<sup>nd</sup> Int. Colloquium on Magnetic Films and Surfaces, Kraków 2015
19. M.Witko "Woman in Science; whether stereotype or feminism", Humboldt-Kolleg Conf. 'Ethics in Science and Life', Toruń 2015
20. M.Witko "Instytut Katalizy i Fizykochemii Powierzchni PAN; Związki Kraków-Lublin", Konf. 40 lat Chemii Teoretycznej na Uniwersytecie Marii Curie-Skłodowskiej - Rozwój i Badania, Lublin 2015

## **Oral presentations**

1. Z.Adamczyk "Protein Adsorption - a True Story", 15<sup>th</sup> European Student Colloid Conf., Krakow 2015
2. Z.Adamczyk "Mechanisms of Nanoparticle Deposition and Stability of Their Monolayers", 10<sup>th</sup> Summer School for Postgraduate Students 'Interfacial Phenomena in Theory and Practice', Sudomie 2015
3. Z.Adamczyk "Mechanizmy zjawisk adsorpcji i osadzania z fazy ciekłej na powierzchniach stałych", Sem. 'Na granicy powierzchni i światła: Adsorpcja i spektroskopia SERS', Kraków 2015
4. P.Batys, M.Nosek, P.Weroniński "Analiza struktury wielowarstw cząstek koloidalnych", Sem. 'Na granicy powierzchni i światła: Adsorpcja i spektroskopia SERS', Kraków 2015
5. Ł.Bratasz, R.Kozłowski, M.Łukomski "Software for a quantitative assessment of risk of damage to objects vulnerable to climate variations", The Getty Conservation Institute Workshop "Epidemiology - basic ideas applied to museum collections", Waddesdon 2015

6. A.Bratek-Skicki, P.Żeliszewska, M.Cieśla, Z.Adamczyk "Określenie mechanizmu adsorpcji fibrynowego na nośnikach koloidalnych", Sem. 'Na granicy powierzchni i światła: Adsorpcja i spektroskopia SERS', Kraków 2015
7. E.Broćławik "Density Functional Theory - basic concepts and applications", Workshop on molecular simulation and drug design, Warszawa 2015
8. E.Broćławik "Electronic structure of bioactive transition metal centers - introduction"; Workshop on molecular simulation and drug design, Warszawa 2015
9. E.Broćławik "Electronic structure of bioactive transition metal centers – advanced topics", Workshop on molecular simulation and drug design, Warszawa 2015
10. E.Broćławik, A.Stępniewski, M.Radoń "Ammonia-modified Co(II) centers in zeolites: spin and electron density redistribution through the CoII-NO bond", 3<sup>rd</sup> Scientific Workshop of the COST Action CM1305 "Explicit control over spin states in technology and Biochemistry, Belgrade 2015
11. E.Broćławik, A.Stępniewski, M.Radoń, K.Góra-Marek "Cobalt sites in zeolites: spin state as the gate controlling charge transfer channels"; 20. Forum Zeolitowe, Stryszawa 2015
12. D.Connell, B.Jachimska, V.A.Ferro, P.Mulheran "Development of a Potential Immunocontraceptive Nanomaterial Using Molecular Dynamics Simulations", Research Presentation Day, Glasgow 2015
13. M.Ćwięka, B.Jachimska "Nondestructive Characterization of Lysozyme Layers on Silica Surface using MP-Surface Plasmon Resonance and Quartz Crystal Microbalance", 15<sup>th</sup> European Student Colloid Conf., Krakow 2015
14. M.Ćwięka, B.Jachimska "LSZ adsorption on silica surface using the QCM-D and MP-SPR", Erasmus+ (KA1 – Mobilność edukacyjna) Meeting, Kraków 2015
15. A.Drelinkiewicz, E.Lalik, R.Kosydar, W.Rojek, T.Szumelda, M.Kołodziej, E.Bielawska "Pasywne autokatalityczne rekombinatory wodoru; idea, wady, zalety", Konf. 'Wybrane aspekty bezpieczeństwa elektrowni jądrowej w Polsce', Mądralin 2015
16. A.Drzewiecka-Matuszek, D.Rutkowska-Żbik, M.Witko "Insight into CpdII oxidation ability towards alcohols and aldehydes – mechanism and ligand effect", 9<sup>th</sup> Int. Symp. 'Surface Heterogeneity Effects in Adsorption and Catalysis on Solids ISSHAC-9', Wrocław 2015
17. M.Elżbieciak-Wodka, K.Kilan, T.Kruk, A.Pajor-Świerzy, K.Podgórska, K.Szczepanowicz, L.Szyk-Warszyńska, P.Warszyński "Nanostructured Materials Based On Polyelectrolyte Multilayers", 10<sup>th</sup> Summer School for Postgraduate Students 'Interfacial Phenomena in Theory and Practice', Sudomie 2015
18. P.Frączek, R.Kozłowski "Hans Mepling *Sąd Ostateczny* – warunki środowiska w otoczeniu dzieła i jego stan zachowania", Symp. 'Wokół tryptyku Hansa Memlinga *Sąd Ostateczny*. Standardy ochrony i wypożyczania unikatowych dzieł sztuki', Gdańsk 2015
19. E.I.García-López, G.Marcì, F.R.Pomilla, L.Palmisano, A.Kirpsza, A.Micek-Ilnicka "Comparison between catalytic and photocatalytic activity in gas-solid regime of semiconductor oxides and carbon nanotubes supported Keggin heteropolyacid", 21<sup>st</sup> Int. Symp. on the Photochemistry and Photophysics of Coordination Compounds, Krakow 2015
20. R.Gryboś, J.Handzlik, F.Tielens "DFT study of Cr, Mo and W oxide monomers supported on silica", 58. Zjazd Polskiego Towarzystwa Chemicznego, Gdańsk 2015
21. A.Y.Gyurova, A.Michna, E.Mileva "Self-assembly of four- and two-antennary oligoglycines in the bulk of aqueous medium", COST Action MP1106 'Smart and green interfaces - from single bubbles and drops to industrial, environmental and biomedical applications (SGI)', Belgrade 2015

22. K.Jóźwiak, K.Pajak, A.Płazińska, W.Płaziński, I.Wainer "Molecular mechanisms of functional selectivity of fenoterol derivatives towards the  $\beta_2$ -adrenergic receptor", 26<sup>th</sup> Int. Symp. on Pharmaceutical and Biomedical Analysis", Tbilisi 2015
23. A.Kędra, R.P.Socha, J.Gurgul, Z.Starowicz, M.Lipiński, S.M.Hanetho, P.Dahl, T.Kruk, K.Łaba, K.Łatka, P.Warszyński "Wykorzystanie efektu plazmonowego na cząstkach metali do wzbudzenia emisji w konwerterach światła", Sem. 'Na granicy powierzchni i światła: Adsorpcja i spektroskopia SERS', Kraków 2015
24. A.Kędra, R.P.Socha, L.Szyk-Warszyńska, M.Zimowska, K.Szczepanowicz, Z.Starowicz, M.Lipiński, K.Łaba, P.Warszyński "Emission of light converters excited by plasmonic particles", 3<sup>rd</sup> Int. Congr. of Energy Efficiency and Energy Related Materials ENEFM2015, Oludeniz 2015
25. A.Kędra, P.Warszyński, R.P.Socha, L.Szyk-Warszyńska, J.Gurgul, K.Szczepanowicz, M.Zimowska, M.Lipiński, S.M.Hanetho, P.Dahl "Synteza i charakteryzacja konwerterów światła opartych na strukturze perowskitu", 6. Symp. 'Fotowoltaika i Transparentna Elektronika', Świeradów-Zdrój 2015
26. K.Kilan, G.J.Koper, P.Warszyński "Effect of cross-linking cations on permeation of alginate containing multilayered membranes", 15<sup>th</sup> Conf. of Int. Assoc. of Colloid and Interface Scientists and 47th Conf. of the German Colloid Society, Mainz 2015
27. H.W.Klemm, G.Peschel, E.Madej, A.Fuhrich, M.Timm, T.Schmidt, H.-J.Freund "Growth of ultrathin Silica Films on Ru(0001)", 79th Annual Meeting of DPG and DPG-Fruhjahrstagung of the Condensed Matter Section, Berlin 2015
28. A.Kornas, R.Grabowski, K.Samson, M.Ruggiero, A.Żelazny, M.Śliwa "Właściwości fizykochemiczne i katalityczne katalizatorów miedziowych w reakcji uwodornienia CO<sub>2</sub> w kierunku eteru dwumetylowego (DME)", 2. Ogólnokrajowa Konf. 'Młodzi Naukowcy w Polsce - Badania i Rozwój', Wrocław 2015
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## 2016

### Plenary, keynote and invited lectures

1. Z.Adamczyk "Mechanisms of noble metal monolayer formation at solid substrates", 11<sup>th</sup> School for Postgraduate Students 'Interfacial Phenomena in Theory and Practice', Sudomie 2016
2. E.Błasiak, S.Łukasiewicz, K.Szczepanowicz, P.Warszyński, M.Dziedzicka-Wasyłewska "Biocompatible polymeric nanoparticles as promising candidates for drug delivery", 2<sup>nd</sup> Central European Biomedical Congr. CEBC, Krakow 2016
3. Ł.Bratasz, R.Kozłowski, M.Łukomski "HERIE – a decision-supporting tool based on quantitative assessment of damage risk", Seminar & Symp. 'The Mechanics of Art Materials and its Future in Heritage Science', The Smithsonian Institution, Washington DC 2016
4. A.Drelinkiewicz, E.Lalik, R.Kosydar "Efekty termiczne reakcji z udziałem wodoru; wyzwanie dla technologii OZE", 3. Ogólnopolskie Forum Chemii Nieorganicznej, Kraków 2016
5. B.Jachimska, K.Tokarczyk "Dendrimers as a platform for designing biologically active carriers", Nanomaterials for Technology Workshop, Glasgow2016
6. D.Jantas, M.Piotrowski, M.Leśkiewicz, M.Regulska, J.Staroń, P.Warszyński, W.Lasoń, K.Szczepanowicz "Neuroprotective activity of (bio)polyelectrolyte-coated nanocapsules containing curcumin", 2<sup>nd</sup> Central European Biomedical Congr. CEBC, Krakow 2016
7. M.Kowacz, M.Marchel, L.Juknaité, J.M.S.S.Esperança, M.J.Romão, A.L.Carvalho, L.P.N.Rebelo, P.Warszyński "Effect of infrared light on protein interfacial water. Consequences for protein self-assembly and protein-surface intercation", 11<sup>th</sup> Conf. on Physics, Chemistry and Biology of Water, Sofia 2016
8. M.Kowacz, M.Marchel, L.Juknaité, A.Mukhopadhyay, A.L.Carvalho, J.M.S.S.Esperança, M.J.Romão, L.P.N.Rebel "Ionic liquids - water interplay in protein crystallization. From additives to nucleants to...", 16<sup>th</sup> Int. Conf. on Crystallization of Biological Macromolecules, Prague 2016
9. R.Kozłowski "Shared understanding facilitates decision making", Global Colloquium of University Presidents 'Preservation of Cultural Heritage: Challenges and Strategies', New Haven. MA 2016
10. R.Kozłowski, A.Kupczak, Ł.Lasyk, A.Działo, Ł.Bratasz, M.Łukomski "HERIE - a web-based software for assessing risk of climate-induced damage to painted wood", Conf. 'Wood Science and Technology II, Microclimates for Panel Paintings', SRAL Art conservation and research, Maastricht 2016
11. K.Malysa "On importance of thin liquid films in the colliding bubble attachment to solid surfaces of different hydrophobicity – a review", Mineral Engineering Conf. MEC2016, Swieradów-Zdrój 2016
12. A.Micek-Ilnicka "Heteropolizwiązki – ich osobliwe właściwości fizykochemiczne, katalityczne i fotokatalityczne", 3. Ogólnopolskie Forum Chemii Nieorganicznej, Kraków 2016

13. T.Pańczyk, Ł.Kończak, P.Wolski "Colloid nanoparticles and carbon nanotubes. What can we learn about their biomedical application from molecular dynamics simulations", Conf. 'Physics of Liquid Matter: Modern Problems PLMMP-2016', Kyiv 2016
14. E.M.Serwicka "Wpływ wykładów Prof. Bielańskiego na formowanie zainteresowań naukowych – refleksja własna", 3. Ogólnopolskie Forum Chemii Nieorganicznej, Kraków 2016
15. Z.Starowicz, H.Kazimierczak, R.P.Socha, K.Berent, M.Lipiński "The effect of the process parameters on microstructure of sliver nanoparticles photochemically deposited on titanium dioxide", 2016 E-MRS Spring Meeting, Lille 2016
16. M.Szaleniec ,A.Rugor, A.Wójcik "Steroid C25 Dehydrogenase, the Bocatalyst for Production of Calcifediol and 25-Hydroxycholesterol", 3<sup>rd</sup> Symp. on Biotransformations for Pharmaceutical and Cosmetic Industry, Warszawa 2016
17. M.Szaleniec, M.Witko, T.Borowski, J.Heider "Is the theoretical modeling a reliable tool for studying the reaction mechanisms of enzymes?", 5<sup>th</sup> Int. Conf. of Biophysics Students, Kraków 2106
18. K.Szczepanowicz, K.Podgórska, M.Piotrowski, P.Warszyński "Synthesis and properties of polyelectrolyte-coated nanocapsules", 2<sup>nd</sup> Central European Biomedical Congr. CEBC, Krakow 2016
19. J.Ślusarczyk, K.Szczepanowicz, M.Leskiewicz, M.Regulska, P.Warszyński, W.Lason, A.Basta-Kaim "Evaluation of protective action of polydatin, free form and in nanocapsules, in the hippocampal organotypic cultures treated with lipopolisaccharide", 2<sup>nd</sup> Central European Biomedical Congr. CEBC, Krakow 2016
20. S.P.de Visser, A.S.Faponle, M.G.Quesne, T.Borowski "Quantum mechanics/molecular mechanics studies of cytochrome P450 peroxygenases for the biosynthesis of biofuels", 16<sup>th</sup> Int. Conf on Theoretical Aspects of Catalysis, Zakopane 2016
21. M.Witko, P.Niemiec, R.Tokarz-Sobieraj, A.Micek-Ilnicka, U.Filek "Catalytic properties of heteropolyacids: theory vs. experiment", 16<sup>th</sup> Int. Congr. on Catalysis, Beijing 2016

## **Oral presentations**

1. E.Bielńska, J.Camra, M.Najbar, A.Weselucha-Birczyńska, T.Wilkosz "Ewolucja katalitycznych warstw tlenkowych aktywnych w bezpośrednim rozkładzie NO na stali austenitycznej AISI 321 pod wpływem czynników zewnętrznych", 48. Ogólnopolskie Kolokwium Katalityczne, Kraków 2016
2. T.Borowski, A.Miłaczewska, Z.Wojdyła "Oxidative C-C bond cleavage by two metalloenzymes and one synthetic complex", Conf. 'Current Trends in Theoretical Chemistry VII', Kraków 2016
3. A.Bratek-Skicki, M.Delcroix, A.van der Straeten, C.Dupont-Gillain "Tunable protein immobilization at interfaces based on polyelectrolyte-protein interactions", Conf. Biointerfaces International 2016, Zurich 2016
4. A.Bratek-Skicki, C.Dupont-Gillain "Selective protein adsorption on stimuli-responsive brushes", 30<sup>th</sup> European Colloid and Interface Society Conf. ECIS 2016, Rome 2016
5. E.Brocławik, T.Borowski, M.Radoń, A.Stępniewski "Stany spinowe i ich znaczenie dla katalizy na centrach metali przejściowych w enzymach i nie tylko", 3. Ogólnopolskie Forum Chemii Nieorganicznej, Kraków 2016
6. E.Brocławik, A.Stępniewski, M.Radoń, K.Góra-Marek "High-level small-scale or periodic DFT modeling for TM centers in zeolites?", Conf. 'Current Trends in Theoretical Chemistry VII', Kraków, 2016
7. M.Duda, A.Rafalska-Łasocha, W.Łasocha "Analiza symetrii ornamentów w polichromiach w kościele mriackim i kościele Franciszkanów w Krakowie", 58. Konwersatorium Krystalograficzne, Wrocław 2016
8. D.Duraczyńska, E.M.Serwicka, A.Michalik-Zym, B.D.Napruszewska, E.Bielńska, R.P.Socha, L.Lityńska-Dobrzyńska "Uniwersalny katalizator typu Ru/SBA-15 do uwodornienia grup C=O, C=C i C≡C", 48. Ogólnopolskie Kolokwium Katalityczne, Kraków 2016

9. M.Gackowski, E.Bielńska, K.Szczepanowicz, P.Warszyński, J.Kryściak-Czerwenka, B.Sulikowski, M.Derewiński "Silica monoliths with deposited zeolite nanoparticles as model, continuous-flow microreactors", 48. Ogólnopolskie Kolokwium Katalityczne, Kraków 2016
10. M.Gackowski, K.Tarach, Ł.Kuterasiński, J.Podobiński, S.Jarczewski, B.Sulikowski, P.Kuśtrowski, J.Datka "Hierarchiczne zeolity Y – materiały o wysokiej kwasowości, porowatości i aktywności katalitycznej", 3. Ogólnopolskie Forum Chemii Nieorganicznej, Kraków 2016
11. A.Kędra, R.Socha, Z.Starowicz, M.Zimowska, M.Lipiński, P.Warszyński "Synthesis and characterization of organic and inorganic perovskites for application in solar cells", Int. Workshop 'Materials and methods for cost-effective solar cell production', Krakow 2016
12. A.Kędra, R.Socha, L.Szyk-Warszyńska, M.Zimowska, Z.Starowicz, M.Lipiński, P.Warszyński "Synteza i charakteryzacja konwerterów światła opartych na strukturze perowskitu", 7. Symp. 'Fotowoltaika i Transparentna Elektronika - Perspektywy Rozwoju', Świeradów-Zdrój 2016
13. K.Kilan, L.Szyk-Warszyńska, G.J.M.Koper, P.Warszyński "Permeability of alginate containing multilayer films cross-linked by multivalent cations", Conf. 'Soft Matter at Aqueous Interface SOMATAI', Crete 2016
14. M.Kołodziej, R.Kosydar, E.Lalik, J.Gurgul, D.Duraczyńska, A.Drelinkiewicz "Activity/selectivity control in  $Pd/H_xMoO_3$  catalyzed cinnamaldehyde and furfural hydrogenation", 48. Ogólnopolskie Kolokwium Katalityczne, Kraków 2016
15. A.Kornas, R.Grabowski, K.Samson, M.Śliwa, D.Rutkowska-Żbik, A.Żelazny, M.Ruggiero "Dimethyl ether synthesis through CO<sub>2</sub> hydrogenation over hybrid catalysts: effects of preparation methods and heteropoly acids", 13<sup>th</sup> Pannonian Int. Symp. on Catalysis, Siofok 2016
16. A.Koziol-Rachwal, T.Ślęzak, B.Matlak, K.Matlak, J. Korecki "Growth and magnetic properties of ultrathin epitaxial FeO films and Fe/FeO bilayers on MgO(001)", 13<sup>th</sup> Joint MMM-Intermag Conf., San Diego CA 2016
17. Z.Krasińska, G.Pathak, L.Szyk-Warszyńska, D.Cakara "Structure investigation of pedot:pss thin films", 11<sup>th</sup> School for Postgraduate Students 'Interfacial Phenomena in Theory and Practice', Sudomie 2016
18. A.Krawczyk, R.Socha, Z.Starowicz, M.Zimowska, M.Lipiński, P.Warszyński "Synthesis and characterization of organic and inorganic perovskites for application in solar cells", Int. Workshop 'Materials and methods for cost-effective solar cell production', Krakow 2016
19. M.Krzan "Influence of bubble wake, its size and shape on the bubble local and terminal velocities", Conf. EuFoam 2016, Dublin 2016
20. M.Krzan "Influence of bubble wake development on bubble motion in surfactant solutions", Symp. SGI-FunC & Conf. COST Smart and Green Interfaces, Athens 2016
21. M.Krzan, E.Jarek, H.Petkova, E.Santini, S.Kudłacik, K.Bialik-Wąs, A.Drabczyk, V.Ungalantha, M.Lofti, A.Javadi, B.Tyliszczak, E.Mileva, P.Warszyński, R.Todorov, F.Ravera, L.Liggieri, R.Miller, D.Exerowa "Piany ciekłe wytworzzone na bazie mieszanin polisacharydów do zastosowań kosmetycznych i biomedycznych", Konf. 'Nowoczesna Kosmetologia – od Nauki od Biznesu', Kraków 2016
22. A.Kupczak, Ł.Lasyk, A.Działo, Ł.Bratasz, M.Łukomski, R.Kozłowski "HERIE - a web-based software for assessing risk of physical damage of heritage objects vulnerable to climate fluctuations", ICOM-CC Joint Interim Meeting 'Physical Issues in the Conservation of Paintings: Monitoring, Documenting and Treatment', Paris 2016
23. A.Kupczak, A.Sadłowska-Sałęga, L.Krzemień, J.Radoń, R.Kozłowski "Modelling impact of collections on indoor climate and energy consumption in libraries and archives", 2<sup>nd</sup> Int. Conf. on Energy Efficiency and Comfort of Historic Buildings, Brussels 2016
24. Ł.Kuterasiński, B.Sulikowski, J.Kryściak-Czerwenka, A.Dziedzicka, K.Durczyk, U.Olsbye, G.Szymański, E.Włoch, E.Bielńska, M.Derewiński "Protonowe centra kwasowe w borokrzemianach o strukturze typu MFI", 48. Ogólnopolskie Kolokwium Katalityczne, Kraków 2016

25. E.Lalik, G.Mordarski, R.P.Socha, A.Drelinkiewicz "Oscillatory mechanism of solid/gas interaction in the palladium/hydrogen system", Int. Discussion on hydrogen energy and applications IDHEA 2016, Nantes 2016
26. D.Lupa, Z.Adamczyk, M.Oćwieja, H.Mrowiec, S.Walas "Kinetyka oksydacyjnego roztwarzania nanocząstek srebra", 59. Zjazd Naukowy PTChem, Poznań 2016
27. D.Lupa, Z.Adamczyk, M.Oćwieja, H.Mrowiec, S.Walas "Mechanisms of oxidative dissolution of silver nanoparticles", 11th School for Postgraduate Students 'Interfacial Phenomena in Theory and Practice', Sudomie 2016
28. J.Maciejewska, K.Kubiak, M.Oćwieja, Z.Adamczyk "Kinetics of gold nanoparticle deposition on PAH-modified gold substrate", 11th School for Postgraduate Students 'Interfacial Phenomena in Theory and Practice', Sudomie 2016
29. J.Maciejewska-Prończuk, Z.Adamczyk, M.Oćwieja, M.Morga "Monowarstwy nanocząstek złota o kontrolowanej strukturze i właściwościach", 59. Zjazd Naukowy PTChem, Poznań 2016
30. M.Nattich-Rak, M.Sadowska, Z.Adamczyk, M.Oćwieja "Mechanizmy osadzania nanocząstek srebra na powierzchni nośników koloidalnych", 59. Zjazd Naukowy PTChem, Poznań 2016
31. P.Niemiec, R.Tokarz-Sobieraj, M.Witko "Catalytic properties of modified heteropolyacids. DFT cluster model study", 16<sup>th</sup> Int. Conf on Theoretical Aspects of Catalysis, Zakopane 2016
32. M.Oćwieja, Z.Adamczyk, J.Maciejewska, K.Kubiak, M.Morga, E.Bielańska, B.Napruszewska "Preparatyka mono- oraz multiwarstw nanocząstek koloidalnych do zastosowań katalitycznych, analitycznych i biobójczych", 48. Ogólnopolskie Kolokwium Katalityczne, Kraków 2016
33. J.Olszówka, R.Karcz, E.Bielańska, R.Dula, J.Kryściak-Czerwenka, A.Michalik-Zym, B.Napruszewska, R.P.Socha, E.M.Serwicka "Utlenie cykloheksanonu do ε-kaprolaktonu przy pomocy nadtlenku wodoru na katalizatorach hydrotalkitowych o różnym stopniu krystaliczności", 48. Ogólnopolskie Kolokwium Katalityczne, Kraków 2016
34. K.Onik, M.Gackowski, E.Bielańska, M.Derewiński, B.Sulikowski "Protozeolitic nanoclusters and mesoporous layered materials prepared from them: physicochemical and catalytic properties", 6<sup>th</sup> Int. Workshop on Layered Materials, Kutná Hora 2016
35. A.Miłaczewska, T.Borowski "Obliczenia metodą hybrydową QM/MM – wgląd w przebieg reakcji katalitycznej metaloenzymu ARD", Dzień Otwarty Cyfronet AGH, Kraków 2016
36. P.Panek, P.Zięba, R.Socha, M.Juel, A.Sypień, K.Gawlińska "In-line processing of n+/p and p/p+ junction systems for cheap crystalline Si solar cells production", Int. Workshop 'Materials and methods for cost-effective solar cell production', Krakow 2016
37. T.Pańczyk, Ł.Kończak, P.Wolski "Carbon nanotubes as pH controlled drugs nanocontainers. Insights from molecular dynamics simulation", World Conf. on Carbon 'Common fundamentals, remarkably versatile applications CARBON 2016', State College PA 2016
38. T.Pańczyk, P.Wolski, Ł.Kończak "A few strategies of using carbon nanotubes as smart drug delivery systems. Insights into mechanisms of action from molecular dynamics simulation", 14<sup>th</sup> Annual Congr. of International Drug Discovery Science and Technology IDDST-South Korea 2016, Gyeonggi 2016
39. W.Płaziński " Activation of the toggle switch and dynamic network of the β2-adrenergic receptor", 8<sup>th</sup> Conversatory of Medicinal Chemistry, Lublin 2016
40. W.Płaziński " Ring inversion properties of hexopyranoses: from force field parametrization to the interplay between ring shape and glycosidic linkage conformation", 8<sup>th</sup> Conversatory of Medicinal Chemistry, Lublin 2016

41. W.Płaziński " Ring inversion properties of hexopyranoses: from force field parametrization to studies on the interplay between ring shape and glycosidic linkage conformation", 28<sup>th</sup> Int. Carbohydrate Symp., New Orleans 2016
42. W.Płaziński, A.Płazińska, M. Drach "Conformational preferences of acyclic aldo- and ketohexoses and their implication for anomeric equilibria", 16<sup>th</sup> Int. Conf on Theoretical Aspects of Catalysis, Zakopane 2016
43. K.Podgórska, K.Szczepanowicz, M.Piotrowski, M.Gajdosova, F.Stepanek, P.Warszyński "Polysaccharide gel nanoparticles for controlled drug delivery and theranostic applications", Int. Conf. & Exhibition NanoTech Poland, Poznań 2016
44. A.Rugor "Oksydoreduktazy ze Sterolibacterium denitrificans jako biokatalizatory do reakcji utleniania pochodnych steroidowych", Dzień Otwarty Cyfronet AGH, Kraków 2016
45. A.Rugor, A.Wójcik, S.Mordalski, J.Staroń, A.Bojarski, M Szaleniec "The propinquity effect in enzyme catalysis: a case study of steroid C25 dehydrogenase", 48. Ogólnopolskie Kolokwium Katalityczne, Kraków 2016
46. A.Rugor, A.Wójcik, S. Mordalski, M.Szaleniec "The mechanism of regioselective hydroxylation of sterols by steroid C25 dehydrogenase", 16<sup>th</sup> Int. Conf on Theoretical Aspects of Catalysis, Zakopane 2016
47. A.Rugor, A.Wójcik, M.Szaleniec "The Mechanism of Regioselective Hydroxylation of Sterols by Steroid C25 Dehydrogenase", 8<sup>th</sup> Int. Congr on Biocatalysis, Hamburg 2016
48. R.Socha "Badania powierzchni krzemu fotowoltaicznego po procesie dotowania z ciekłych źródeł", 7. Symp. 'Fotowoltaika i Transparentna Elektronika - Perspektywy Rozwoju', Świebodz-Zdrój 2016
49. R.P.Socha, A.Kędra, M.Zimowska, P.Panek,M.Lipiński, P.Warszyński "Surface chemistry of silicon texturized with HF", 18<sup>th</sup> European Symp. on Fluorine Chemistry, Kyiv 2016
50. R.Socha, P.Panek "Studies of the silicate glass formed on the silicon surface during inline solar cell fabrication", Int. Workshop 'Materials and methods for cost-effective solar cell production', Krakow 2016
51. R.P.Socha, P.Panek "Studies of the Silicate Glasses Formed on the Silicon Surface During in-Line Solar Cell Fabrication", 8<sup>th</sup> European Silicon Days, Poznań 2016
52. Z.Starowicz, A.Kędra, K.Berent, K.Gawlińska, K.Gwóźdź, E.Zielony, G.Kulesza-Matlak, R.P.Socha, K.Drabczyk, M.Lipiński "Experimental and simulation studies of optimal plasmonic structure for the front side configuration of silicon solar cells and photodiodes", Int. Workshop 'Materials and methods for cost-effective solar cell production', Krakow 2016
53. A.Stępniowski, E.Brocławik, M.Radoń, K.Góra-Marek "Description of Co-NO bond in zeolites: DFT and CASSCF calculations", 48. Ogólnopolskie Kolokwium Katalityczne, Kraków 2016
54. A.Stępniowski, E.Brocławik, M.Radoń, K.Góra-Marek "Large versus small-scale modeling for TM centers in catalysis: is bigger always better?", Conf. 'Modeling & Design of Molecular Materials', Trzebnica 2016
55. M.Strojecki, A.Mleczkowska, Ł.Bratasz, R.Kozłowski "Particle deposition and sources in the indoor environment of historic churches", 12<sup>th</sup> Int. Conf. 'Indoor Air Quality - in Heritage and Historic Environments', Birmingham 2016
56. M.Szaleniec "Biokataliza i mikrobiologia dla różnych dziedzin przemysłu", Dzień Otwarty Klastra Life Science, Kraków 2016
57. M.Szaleniec, J.Heider "Elucidation of Factors Responsible for Enantiospecificity in Radical C-C Coupling Catalyzed by Benzylsuccinate Synthase", 8<sup>th</sup> Int. Congr on Biocatalysis, Hamburg 2016
58. M.Szczęch, O.Marszałek, M.Piotrowski, D.Jantas, K.Szczepanowicz, P.Warszyński "Biopolymer nanoparticles as neuroprotectants-loaded carriers for drug delivery to the brain", Int. Conf. & Exhibition NanoTech Poland, Poznań 2016

59. S.Świątek, B.Jachimska "Funkcjonalizacja powierzchni złota poprzez adsorpcję wołowej  $\beta$ -laktoglobuliny", Konf. 'Nanobiomateriały - teoria i praktyka', Toruń 2016
60. K.Tarach, M.Gackowski, B. Sulikowski, S. Jarczewski, P.Kuśtrowski, J. Datka "Hierarchical zeolites FAU: porosity, acidity and catalytic properties", 13<sup>th</sup> Pannonian Int. Symp. on Catalysis, Siofok 2016
61. K.Tokarczyk, B.Jachimska Towards modern drug carriers: Immobilization of PAMAM dendrimers on solid support", Kuźnia Młodych Talentów Akademii Młodych Uczonych PAN, Jabłonna 2016
62. R.Tokarz-Sobieraj, P.Niemiec, M.Witko "Heteropolikwasy modyfikowane w pozycji atomu addenda. Obliczenia DFT", 3. Ogólnopolskie Forum Chemii Nieorganicznej, Kraków 2016
63. P.Warszyński "Nanoparticulate delivery systems for therapies against neurodegenerative diseases", Conf. of Polish Norwegian Research Programme 'Together for Innovation in Health', Krakow 2016
64. A.Wiertel, C.Karaguzel, J.Zawała, O.Sahbaz, K.Małysa " Effect of CTAB concentration on kinetics of bubble attachment and quartz flotation", 11<sup>th</sup> School for Postgraduate Students 'Interfacial Phenomena in Theory and Practice', Sudomie 2016
65. A.Wiertel, J.Zawała, K.Małysa, " On mechanism of the three-phase contact formation during bubble collision with quartz surface in CTAB solutions", 59. Zjazd Naukowy PTChem, Poznań 2016
66. M.Witko "Jerzy Haber Institute of Catalysis and Surface Chemistry PAS", Polish-French Scientific Workshop on Life Sciences, Kraków 2016
67. M.Włodek, M.Kolasińska-Sojka, M.Szuwarzynski, P.Warszyński "Effect of Quantum Dots size on their incorporation into POPC/POPE supported lipid bilayers in dependence of the cushion polyelectrolyte multilayers", 30<sup>th</sup> European Colloid and Interface Society Conf. ECIS 2016, Rome 2016
68. M.Włodek, M.Kolasińska-Sojka, M.Szuwarzynski, S.Zapotoczny, R.von Klitzing, P.Warszyński "Effect of Vesicle Deposition Conditions and Surface Properties of the Cushion Material on Formation of POPC/POPE Supported Lipid Bilayer", Bristol PhD Day, University of Bristol, Bristol 2016
69. J.Zawała, D.Kosior, P.B.Kowalcuk, J.Drzymała, K.Małysa "Modelling of influence of adsorption layer on kinetics of bubble collisions and attachment to hydrophobic solid", 11<sup>th</sup> School for Postgraduate Students 'Interfacial Phenomena in Theory and Practice', Sudomie 2016
70. J.Zawała, P.B.Kowalcuk, D.Kosior, J.Drzymala, K.Małysa "A Correlation Between Kinetics of Bubble Attachment to Solids and Flotation Efficiency", Symp. SGI-FunC & Conf. COST Smart and Green Interfaces, Athens 2016
71. M.Zimowska, L.Lityńska-Dobrzyńska, J.Gurgul, R.P.Socha, H.Pálková, L.Matachowski, K.Łątka "Influence of surface composition of Fe-doped porous clay heterostructures on catalytic properties", 8<sup>th</sup> Mid-European Clay Conf. MECC 2016, Kosice 2016
72. A.Żelazny, R.Grabowski, M.Śliwa, M.Ruggiero, K.Samson, A.Kornas, D.Duraczyńska, K.Gołąbek "Cu/MxOy catalysts for glycerol hydrognolysis. Influence of the preparation method and sodium hydroxide addition", 13<sup>th</sup> Pannonian Int. Symp. on Catalysis, Siofok 2016
73. P.Żeliszewska, M.Wasilewska, Z.Adamczyk, A.Bratek-Skicki "Mechanisms of fibrinogen adsorption on colloid microparticles", 30<sup>th</sup> European Colloid and Interface Society Conf. ECIS 2016, Rome 2016

## **Conferences and scientific events organized by the Institute**

### **2014**

1. 46. Ogólnopolskie Kollokwiunum Katalityczne, Kraków, 19-21 marca 2014 (B.Sulikowski)
2. Festiwal Nauki "Z nauką przez wieki", Rynek Główny, Kraków 21-24 maja 2014 (N.Spiridis)
3. 3<sup>rd</sup> International Symposium on Air & Water Pollution Abatement Catalysis, Krakow, September 1<sup>st</sup>-5<sup>th</sup>, 2014 (M.Witko)
4. Seminarium Sprawozdawcze POIG FUNANO, Kraków, 21 października 2014 (Z.Adamczyk)
5. 5<sup>th</sup> Meeting X-ray and other techniques in investigations of the objects of cultural heritage, Krakow, May 14<sup>th</sup>-17<sup>th</sup>, 2014 (z Uniwersytetem Jagiellońskim) (R.Kozłowski, W.Łasocha)
6. International Symposium on Clean Energy from Ethanol, Rzeszów, July 28<sup>th</sup>-31<sup>st</sup>, 2014 (z Uniwersytetem Rzeszowskim) (A.Kowal)
7. Dzień Otwarty IKiFP PAN, Kraków, 7 listopada 2014 (M.Nattich-Rak)

### **2015**

1. 47. Ogólnopolskie Kollokwiunum Katalityczne, Kraków, 16-18 marca 2015 (B.Sulikowski)
2. Festiwal Nauki "Oświeć się!", Rynek Główny, Kraków 20-23 maja 2015 (N.Spiridis)
3. 15th European Student Colloid Conference, Kraków, 8-11 czerwca 2015 (P.Warszyński)
4. Seminarium 'Na granicy powierzchni i światła: Adsorpcja i Spektroskopia SERS', Kraków, 2-3 lipca 2015 (Z.Adamczyk)
5. 9th International Symposium 'Surface Heterogeneity Effects in Adsorption and Catalysis on Solids', Wrocław, 7-23 lipca 2015 (M.Witko, R.Tokarz-Sobieraj)
6. 4th International Symposium on Surface Imaging / Spectroscopy at the Solid / Liquid Interface, Kraków, 2-4 września 2015 (P.Warszyński)
7. Polish-American Innovation Bridge PAIB/PAMI: How to begin, Kraków 20-21 września 2015 (B.Jachimska)
8. Workshop 'Suspensions – designing, synthesis, properties, application SUSPENS', Kraków, 25 września 2015 (Z.Adamczyk)
9. Dzień Otwarty IKiFP PAN, Kraków, 6 listopada 2015 (R.Kozłowski)
10. Warsztat "Wpływ ogrzewania zabytkowych kościołów na przenoszenie i osadzanie pyłów", Warszawa, 13 listopada 2015 (R.Kozłowski)

### **2016**

1. 48. Ogólnopolskie Kollokwiunum Katalityczne, Kraków, 16-18 marca 2016 (B.Sulikowski)
2. 6<sup>th</sup> Meeting 'X-ray and other techniques in investigations of the objects of cultural heritage', Krakow, May 19<sup>th</sup>-21<sup>st</sup>, 2016 (R.Kozłowski, W.Łasocha)
3. Festiwal Nauki "Czas i przestrzeń", Rynek Główny, Kraków 19-21 maja 2016 (N.Spiridis)

4. 16th International Conference on Theoretical Aspects of Catalysis ICTAC-16, Zakopane, June 19<sup>th</sup>-23<sup>rd</sup>, 2016 (M.Witko)
5. International QCM-D Workshop “Functional coatings using QCM-D system: theory and practice”, Krakow, June 30<sup>th</sup>, 2016 (B.Jachimska)
6. International Workshop “Materials and methods for cost-effective solar cell production” InLinePV Project Workshop, Krakow, November 16<sup>th</sup>, 2016 (P.Warszyński, R.Socha)
7. Dzień Otwarty IKiFP PAN, Kraków, 25 listopada 2016 (M.Nattich-Rak)