JAGIELLONIAN UNIVERSITY

Faculty of Chemistry

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Address:
30-060 Kraków, Ingardena 3
Poland
Tel: +48-12-663 22 15
Fax: +48-12-634 05 15

Editors: Barbara Krajewska, Dr habil; Professor Edward Mikuli
Photographs: Paweł Bernard, MSc; Tomasz Dybiec, MSc (front cover)

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Back cover: Jagiellonian University coat of arms from Collegium Novum

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KRAKÓW AND ITS UNIVERSITY

'Cracovia totius Poloniae urbs celeberrima' – 'Kraków, Poland's most glorious city' – the former capital of Poland, one of the oldest and most beautiful cities of Central Europe included by UNESCO in the list of World Heritage Sites, throughout centuries has grown to be a symbol of Polish tradition, culture and national identity. The city throve in the Middle Ages leaving impressive traces of its splendour and wealth: the Old Town with the largest mediaeval market square in Europe, the beautiful Renaissance Wawel Royal Castle and the famous Jagiellonian University. The University – Alma Mater Cracoviensis – was founded by King Casimir the Great in 1364 as Kraków Academy. Later, to commemorate Queen Jadwiga and her husband King Vladislaus Jagiello, the benefactors of its renewal in 1400, the Academy was renamed the Jagiellonian University.

Integrated with Kraków, its people and fate, the Jagiellonian University rendered the city a centre of learning and science, culture and art, a centre of thought that was famous across the whole of Europe. 'Plus ratio quam vis' – 'Reason more than force' – reads the motto of the University. For over six centuries the University has carried out its mission welcoming all seeking an education, among its most illustrious students being Nicolaus Copernicus and Karol Wojtyła.

Along with other institutions of higher education the Jagiellonian University now make Kraków Poland's second largest academic centre. At present the University has fifteen faculties: Law and Administration; Medicine; Pharmacy; Health Sciences; Philosophy; History; Philology; Polish Studies; Physics, Astronomy and Applied Computer Science; Mathematics and Computer Science; Chemistry; Biology and Earth Sciences; Management and Social Communication; International and Political Studies; Biochemistry, Biophysics and Biotechnology. It employes 3650 academic teachers, among them 1000 professors and doctores habilitati. The present number of students that includes intra- and extra-mural students, and PhD and post-graduate students amounts to 46500.

Barbara Krajewska

Collegium Novum

CHEMISTRY IN THE JAGIELLONIAN UNIVERSITY

The first chair of chemistry in the Jagiellonian University was established at 1782. It was also the first such chair in Poland. Originally belonging to the Faculty of Medicine, later on to the Faculty of Philosophy and subsequently to the Faculty of Mathematics, Physics and Chemistry, in 1981 the chair was upgraded to an independent Faculty of Chemistry. The best known among chemists who have worked at the Jagiellonian University are Karol Olszewski (1846–1915) who was the first to liquefy oxygen, nitrogen and carbon monoxide, and Bohdan Szyszkowski (1873–1931) known for the equation that correlates surface tension and concentration.

Currently, 173 academic teachers work at the Faculty, among them the number of the senior academic staff that comprises professors of chemistry, associate professors and doctores habilitati amounts to 62. The Faculty is entitled to award licentiate, MSc, PhD and Doctor habilitatus degrees. The Faculty offers courses in chemistry, environmental protection and in advanced materials and nanotechnology with total number of students reaching 1000.

Faculty of Chemistry

Faculty authorities

Dean	Professor Grażyna Stochel
Vice-Dean for Research and Cooperation	Professor Zbigniew Sojka
Vice-Dean for General Affairs	Barbara Rys, Dr habil
Vice-Dean for Students Affairs	Professor Artur Michalak

Departments and research groups

Department of Analytical Chemistry
- Chemometrics – Professor Andrzej Parczewski
- Analytical Flow Techniques – Professor Paweł Kościelniak

Department of Chemical Education – Professor Anna Migdał-Mikuli

Department of Chemical Physics:
- Phase Transitions – Professor Edward Mikuli
- Vibrational Spectroscopy – Professor Leonard Proniewicz

Department of Chemical Technology:
- Catalytic Environmental Technologies – Lucjan Chmielarz, Dr habil
- Chemistry of Polymers – Professor Edgar Bortel
- Technology of Materials and Nanomaterials – Professor Roman Dziembaj
- Organic Technology – Piotr Kuśtrowski, Dr habil

Department of Computational Methods in Chemistry – Andrzej Eilmes, Dr habil

Department of General Chemistry:
- Environmental Chemistry – Professor Adam Juszkiewicz
- Physicochemistry of Interfacial Phenomena – Professor Patrycja Dynarowicz-Łątka

Department of Inorganic Chemistry:
- Coordination and Bioinorganic Physicochemistry – Professor Grażyna Stochel
- Coordination Chemistry – Janusz Szklarzewicz, Dr habil
- Environmental Catalysis – Professor Mieczysława Najbar
- Cryogenics and Food Chemistry – Maria Łabanowska, Dr habil
- Inorganic Molecular Materials – Professor Barbara Sieklucka
- Kinetics of Heterogeneous Reactions – Joanna Łojewska, Dr habil
- Catalysis and Solid State Chemistry I – Professor Zbigniew Sojka
- Zeolites – Professor Jerzy Datka
- Materials and Surface Chemistry – Andrzej Kotarba, Dr habil
- Catalysis and Solid State Chemistry II – Wacław Makowski, Dr habil

Department of Crystal Chemistry and Crystal Physics:

Crystal Chemistry of Drugs – Professor Barbara Oleksyn
Crystal Structure Analysis – Professor Katarzyna Stadnicka
Physical Crystallography – Professor Stanisław Hodorowicz
Protein Crystallography – Krzysztof Lewiński, Dr habil
Structural-Oriented Powder Diffractometry – Professor Wiesław Łasocha

Department of Organic Chemistry:

Chemistry of Carbocyclic Compounds – Janusz Sepioł, Associate Professor
Organic Physicochemistry – Barbara Rys, Dr habil
Organic Stereochemistry – Janusz Jamrozik, Dr habil
Chemistry of Heterocyclic Compounds – Anna Kolasa, PhD
Supramolecular and Biomimetic Chemistry – Julita Eilmes, Dr habil

Department of Physical Chemistry and Electrochemistry:

Electrochemistry – Marian Jaskuła, Dr habil
Femtochemistry – Marek Mac, Dr habil
Molecular Spectroscopy – Professor Marek Wójcik
Nanotechnology of Polymers and Biomaterials – Professor Maria Nowakowska
Photochemistry and Luminescence Research – Professor Jan Najbar
Physical Chemistry of Surfaces – Professor Maria Paluch

Department of Theoretical Chemistry:

Quantum Chemistry – Professor Roman Nalewajski
Organic Semiconductors – Professor Piotr Petelenz
Theoretical Molecular Physics – Professor Marek Pawlikowski
Thermodynamics and Dynamics of Chemical Reactions – Marek Frankowicz, Dr habil

Senior Academic Staff

Małgorzata Barańska

Dr habil, PhD

Research profile

Molecular spectroscopy; Raman and IR spectroscopy; Mapping and imaging; Quantum-chemical calculation; Bioactive compounds; Drugs; Secondary plant metabolites

Professional Qualifications: Habilitation, 2007, "Application of Raman mapping to *in situ* analysis of plant bioactive compounds"; PhD, 1999, "Molecular structure study on cimetidine and famotidine and their complexes with some metal ions by spectroscopy methods"; MSc (completed with honors), 1992, "Oxidation of methane on Pd/SiO2 detected by chromatography and mass spectrometry methods". Awarded for scientific achievements with prizes of the Jagiellonian University Rector (2008, 2007, 2004) and of the Ministry of Higher Education (2005). Associate Professor since 2007 and Scientific Secretary of the Faculty of Chemistry since 2008.

In my research I apply the infrared absorption spectroscopy and Raman scattering spectroscopy to study the molecular structures of bioactive compounds, their derivatives and complexes with metal ions. As supplementary methods, nuclear magnetic resonance spectroscopy and electron absorption spectroscopy are used. To interpret obtained experimental results I carry out the quantum-chemical calculations and molecular modelling. My research is focused on some important plant components contributing to health and sensory properties of plant food as well as drugs and potentially active compounds.

Selected publications

1. Barańska M., Schulz H., Schütze W., Determination of lycopene and β-carotene content in tomato fruits and related products: a comparison of FT-Raman, ATR-IR and NIR spectroscopy, Anal. Chem., 78, 8456–8461, 2006.
2. Barańska M., Schulz H., Joubert E., Manley M., *In situ* flavonoids analysis by FT-Raman spectroscopy: identification, distribution and quantification of aspalathin in green rooibos (Aspalathus linearis), Anal. Chem., 78, 7716–7721, 2006.
3. Barańska M., Barański R., Schulz H., Nothnagel T., Tissue specific accumulation of carotenoids in carrot roots, Planta, 224, 1028–1037, 2006.
4. Barańska M., Schulz H., Christensen L., Structural changes of polyacetylenes in ginseng root can be observed *in situ* by Raman spectroscopy, J. Agric. Food Chem., 54, 3629–3635, 2006.
5. Barańska M., Schulz H., Spatial tissue distribution of polyacetylenes in carrot root, Analyst, 130, 855–859, 2005.
6. Barańska M., Schulz H., Siuda R., Strehle M.A., Rösch P., Popp J., Joubert E., Manley M., Quality control of *Harpagophytum Procumbens* and its related phytopharmaceutical products by means of NIR-FT-Raman spectroscopy, Biopolymers, 77, 1–8, 2005.

Marek Boczar

Dr habil, PhD

Research profile

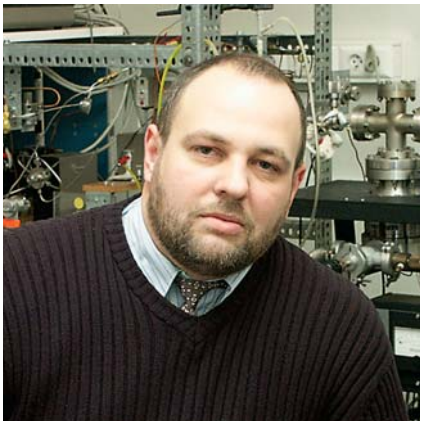
Major fields: Molecular spectroscopy; Theory of the infrared spectra; Hydrogen bonds; Fine structure of X-H bands in hydrogen bonded systems; Adiabatic approximation in vibrational calculations; Resonance interaction; Fermi resonance; Isotopic effects; Shapes and widths of infrared bands; Vibrational spectra of nucleic acid bases; Ab inito calculation in the ground and excited states of molecules; Theory of multidimensional proton tunneling; Coupling of hindered rotation with vibrations and electronic states in molecules with CH_3 groups; Factor analysi;. Zeolites; Heterogeneity of OH groups in zeolites.

Selected publications

1. Kwiendacz J., Boczar M., Wójcik M.J., Theoretical and spectroscopic study of infrared spectra of hydrogen-bonded 2,4-dithiouracil crystal and its deuterated derivative, Polish J. Chem., 83, 895–915, 2009.
2. Wójcik M.J, Boda Ł., Boczar M., Theoretical study of proton tuneling in the excited state of tropolone, J. Chem. Phys., 130, 164306, 2009.
3. Boczar M., Kwiendacz J., Wójcik M.J.,Theoretical and spectroscopic study of infrared spectra of hydrogen-bonded 1-methyluracil crystal and its deuterated derivative, J. Chem. Phys., 128, 164506, 2008.
4. Boczar M., Boda Ł., Wójcik M.J., Theoretical modeling of O-H stretching IR bands of hydrogen-bonded dimers of benzoic acid in S0 and S1 electronic states, J. Chem. Phys., 127, 084307, 2007.
5. Boczar M., Wójcik M.J., Boda Ł., Theoretical model for a tetrad of hydrogen bonds and its application to interpretation of infrared spectra of salicylic acid, J. Chem. Phys., 124, 084306, 2006.
6. Boczar M., Wójcik M.J., Boda Ł., Theoretical model of infrared spectra of hydrogen bonds in molecular crystals and its application to interpretation of infrared of 1-methylthymine, J. Chem. Phys., 125, 084709, 2006.
7. Boczar M., Wójcik M.J., Boda Ł., Theoretical modeling of infrared spectra of hydrogen-bonded crystals of salicylic acid, Spectrochim. Acta, 64, 757–760, 2006.
8. Boczar M., Boda Ł., Wójcik M.J., Theoretical modeling of N-H and N-D stretching bands of hydrogen-bonded 1-methylthymine crystal and its deuterated form, Comput. Lett., 2, 205–219, 2006.

Lucjan Chmielarz

Dr habil, PhD



Research profile

Environmental and industrial catalysis; Solid state chemistry; Microporous and mesoporous ordered materials

Habilitation, 2007, Jagiellonian University
PhD, 1997, Jagiellonian University
MSc, 1992, Jagiellonian University

Coordinator of the Course of Studies in Environmental Protection at the Jagiellonian University (since 2008); Head of the Catalytic Environmental Technologies research group (since 2008).

Main research topics: Catalytic reduction and decomposition of nitrogen oxides; Catalytic incineration of ammonia and VOCs; Synthesis and functionalization of catalytic systems based on cationic layered clays (e.g. PILCs, PCHs), anionic clays (LDHs) and mesoporous silica.

Methods: Chemical analysis (EPMA); Structure (XRD, UV-vis-DRS); Texture (BET); Thermal stability (TG-QMS, DTA); Surface acidity/basicity (NH_3-/CO_2-TPD); Redox properties (TPRed/Ox); Catalytic tests (GC-TCD-FID, QMS).

International cooperation: University of Antwerp, Belgium; Technical University of Ostrava, Czech Republic; S&B Industrial Minerals GmbH, Germany.

Selected publications

1. Chmielarz L., Kuśtrowski P., Zbroja M., Gil-Knap B., Datka J., Dziembaj R., SCR of NO by NH_3 on alumina or titania pillared montmorillonite modified with Cu or Co. Part II Temperature programmed studies, Appl. Catal., B 53, 47–61, 2004.
2. Chmielarz L., Kuśtrowski P., Zbroja M., Łasocha W., Dziembaj R., Selective reduction of NO with NH_3 over pillared clays modified with transition metals, Catal. Today, 90 43–49, 2004.
3. Chmielarz L., Kuśtrowski P., Rafalska-Łasocha A., Dziembaj R., Selective oxidation of ammonia to nitrogen on transition metal containing mixed metal oxides, Appl. Catal. B, 58, 235–244, 2005.
4. Kuśtrowski P., Chmielarz L., Dziembaj R., Cool P., Vansant E.F., Modification of MCM-48-, SBA-15-, MCF- and MSU-type mesoporous silicas with transition metals using the molecular designed dispersion method, J. Phys. Chem. B, 109, 11552–11558, 2005.
5. Chmielarz L., Kuśtrowski P., Dziembaj R., Cool P., Vansant E.F, Catalytic performance of the various mesoporous silicas modified with copper or iron oxides introduced by different methods in the selective reduction of NO by ammonia, Appl. Catal. B, 62, 369–380, 2006.
6. Chmielarz L., Kuśtrowski P., Drozdek M., Dziembaj R., Cool P., Vansant E.F, Selective catalytic oxidation of ammonia into nitrogen over PCH modified with copper and iron species, Catal. Today, 119**,** 181–186, 2007.
7. Chmielarz L., Kuśtrowski P., Michalik M., Dudek B., Piwowarska Z., Dziembaj R., Vermiculites intercalated with Al_2O_3 pillars and modified with transition metals as catalysts of DeNOx process, Catal. Today, 137, 242–246, 2008.

Jerzy Datka

Professor of Chemistry, Dr habil, PhD

Research profile

IR spectroscopy; Active sites on catalysts; Zeolites

My research activity is related to IR spectroscopic studies of active sites on the surfaces of catalysts, zeolites in particular, these being of importance in refinery and „fine chemistry" industry. In our IR investigations, the properties of active sites in zeolites and their interactions with reactant molecules are complemented with quantum chemistry calculations. One subject of our research is acid sites in zeolites, these being catalysts of industrially most important reactions. Another subject is transition metal cations in zeolites, these by contrast being catalysts of redox reactions. Our research group has published over 200 papers in international journals, the number of their citations being over 2200 (h-index of 26). We have realized over ten national and international research grants and have visited a number of foreign laboratories as experts in IR spectroscopy, at the same time having visitors from many Polish and foreign laboratories coming for the IR spectroscopy expertise to be applied to the problems of catalysis and the chemistry of zeolites.

Selected publications

1. Datka J., Kukulska-Zając E., IR Studies of the activation of C=C bond in alkenes by Cu^{+} ions in zeolites, J. Phys. Chem. B, 108, 11760, 2004.
2. Aurault P., Datka J., Laforge S., Martin D., Guisnet M., Characterization of internal and external acidity of H-MCM-22 zeolites, J. Phys. Chem. B, 108, 13755–13766, 2004.
3. Brocławik E., Rejmak P., Kozyra P., Datka J., DFT quantum chemical modeling of the interaction of alkenes with Cu^{+} sites in zeolites, Catal. Today, 114, 162–167, 2006.
4. Góra-Marek K., Datka J. Dźwigaj S. Che M., IR studies of nature of active centers in vanadosilicates, J. Phys. Chem., 110, 6763–6767, 2006.
5. Kukulska-Zając E., Datka J. The transformations of formaldehyde molecules in CuZSM-5 zeolites, J. Phys. Chem, 111, 3471–3475, 2007.
6. Gil B, Mierzyńska K., Szczerbińska M., Datka J., Basic sites in zeolites followed by IR studies of NO^{+}, Appl. Catal., 319, 64–71, 2007.
7. Gil B., Góra-Marek K., Datka J., Quantitative IR studies of the concentration of Co^{2+} and Co^{3+} in zeolites CoZSM-5 and CoFER, Appl. Catal., 353, 117–122, 2008.
8. Rejmak P., Brocławik E., Góra-Marek K., Radoń M., Datka J., Nitrogen monoxide interaction with Cu(I) sites in zeolites X and Y: quantum chemical calculations and IR studies, J. Phys. Chem.,112, 17998–18010, 2008.

Patrycja Dynarowicz-Łątka

Professor of Chemistry, Dr habil, PhD

Research profile

Physical chemistry of interfaces; Surface chemistry

My research is focused on the properties of gas-liquid and gas-solid interfaces, with interest on:

1. Highly ordered organic thin films. Using Langmuir-Blodgett deposition and self-assembly, films can be formed as thin as a single molecular layer with very good control over structure. Highly ordered, defect-free films with controllable molecular orientation and architecture can thus be fabricated and applied in optical and molecular electronic devices and in highly specific chemical sensors.

2. Molecular interactions in monolayers. In this area of research cellular membranes are modelled with Langmuir monolayers and the interactions between membrane components and various biomolecules are investigated. The work involves polyene antibiotics (amphotericin B, nystatin) and new generation anticancer drugs (miltefosine, edelfosine), and is done to gain understanding of their mode of action at membrane level.

3. Synthesis and physico-chemical characterization of surface active molecules. In this project novel surfactants of classical amphiphilic structure as well as non-typical surface active compounds (e.g. di- or tri-block semifluorinated alkanes) are synthesized. For their characterization various optical and spectroscopic methods are used.

Selected publications

1. Broniatowski M., Dynarowicz-Łątka P., Semifluorinated alkanes – primitive surfactants of fascinating properties, Adv. Colloid Interfac. Sci., 138, 63–83, 2008.
2. Broniatowski M., Dynarowicz-Łątka P., Interactions of a fluoroaryl surfactant with hydrogenated, partially fluorinated and perfluorinated surfactants at the air/water interface, Langmuir, 22, 6622–6628, 2006.
3. Hąc-Wydro K., Dynarowicz-Łątka P., Interaction between nystatin and natural membrane lipids in Langmuir monolayers – the role of phospholipids in the mechanism of polyene action, Biophys. Chem., 123, 154–161, 2006.
4. Broniatowski M., Vila Romeu N., Dynarowicz-Łątka P., Langmuir monolayer characteristics of a perfluoroaryl surfactant: 10-perfluorobenzyl-decane-1-ol (PBD), J. Fluorine Chem., 127, 909–915, 2006.
5. Hąc-Wydro K., Dynarowicz-Łątka P., Grzybowska J., Borowski E., N-(1-piperidine propionyl)amphotericin B metyl ester (PAME) – a new derivative of the antifungal antibiotic – amphotericin B: searching for the mechanism of its reduced toxicity. The Langmuir monolayer study, J. Colloid Interfac. Sci., 287, 476–484, 2005.
6. Dynarowicz-Łątka P., Seoane R., Miñones J., Velo M., Study of penetration of amphotericin B into cholesterol or ergosterol containing dipalmitoyl phosphatidylcholine Langmuir monolayers, Colloid. Surface. B, 27, 249–263, 2002.
7. Dynarowicz-Łątka P., Dhabanalan A., Oliveira ON., Modern physicochemical research on Langmuir monolayer, Adv. Colloid Interfac. Sci., 91, 221–293, 2001.

Roman Dziembaj

Professor of Chemistry, Dr habil, PhD

Research profile

Catalysis; Solid state chemistry; Materials science and technology; Surface spectroscopy; Thermal analysis and calorimetry

Head of the Chemical Technology Department and of the Technology of Materials and Nanomaterials research group; Organizer and Head of two other groups (Catalysis & Solid State Chemistry II, Industrial Catalysts & Adsorbents) and ESCA and Thermal Analyses & Calorimetry Laboratories; Former Dean of the Faculty of Chemistry; Humboldt Foundation Fellow; Four of the PhD holders who completed the degree under his supervision are now habilitated and have their individual research groups.

Previously his research activities were concerned with transition metals and their oxide systems as catalysts. The activities were extended later to preparation, characterization and application of other types of materials, composites and nanomaterials fabricated from carbons, natural clays, synthetic layered materials and polymers. The total number of his publications exceeds 230.

Selected publications

1. Bielański A., Dziembaj R., Małecka-Lubańska A., Poźniczek J., Hasik M., Drozdek M., Polyaniline supported heteropolyacid ($H_4SiW_{12}O_{40}$) as the catalyst for MTBE synthesis, J. Catal., 185, 363–370, 1999.
2. Chmielarz L, Kuśtrowski P., Zbroja M., Gil-Knap B., Datka J., Dziembaj R., SCR of NO by NH_3 on alumina or titania pillared montmorillonite various modified with Cu or Co. Part II. Temperature programmed studies, Appl. Catal. B: Environ., 53, 47–61, 2004.
3. Kuśtrowski P., Sułkowska D., Chmielarz L., Rafalska-Łasocha A., Dudek B., Dziembaj R., Influence of thermal treatment conditions on the activity of hydrotalcite-derived Mg-Al oxides in the aldol condensation of acetone, Micropor. Mesopor. Mat., 78, 11–22, 2005.
4. Kuśtrowski P., Chmielarz L., Dziembaj R., Cool P., Vansant E.F., Dehydrogenation of ethylbenzene with nitrous oxide in the presence of mesoporous silica materials modified with transition metal oxides, J. Phys. Chem. A, 109, 330–336, 2005.
5. Kuśtrowski P., Chmielarz L., Dziembaj R., Cool P., Vansant E.F., Modification of MCM-48-, SBA-15-, MCF- and MSU-type mesoporous silicas with transition metal oxides using the molecular designed dispersion method, J. Phys. Chem. B, 109, 11552–11558, 2005.
6. Segura Y., Cool P., Kuśtrowski P., Chmielarz L., Dziembaj R., Vansant E.F., Characterization of vanadium and titanium oxide supported SBA-15, J. Phys. Chem. B, 109, 12071–12079, 2005.
7. Molenda M., Dziembaj R., Podstawka E., Proniewicz L.M., Piwowarska Z., An attempt to improve electrical conductivity of pyrolysed carbon-LiMn2O4-ySy (0≤y≤0.5) composites, J. Power Sources, 174, 613–618, 2007.

Andrzej Eilmes

Dr habil, PhD

Research profile

Excitons in molecular crystals; Effects of disorder in molecular systems; Charge transport in polymers and polymer electrolytes

Research interests include theoretical investigations of Frenkel and charge-transfer excitons in molecular crystals (oligoacenes, fullerene) and charge transport in molecular materials (polymers). Particular attention is paid to manifestations of energetic and orientational disorder in spectroscopy (absorption, electroabsorption, second-harmonic generation) and in transport properties of such systems.

Current research focuses on theoretical description of ion transport in polymer-based solid electrolytes and on solvent effects on ion complexation. Computational methods used in modelling include quantum-chemical calculations and molecular dynamics simulations.

Selected publications

1. Eilmes A., Römer R.A., Schreiber M., The two-dimensional Anderson model of localization with random hopping, Eur. Phys. J. B, 1, 29–38, 1998.
2. Eilmes A., Fischer A.M., Römer R.A., Critical parameters for the disorder-induced metal-insulator transition in fcc and bcc lattices, Phys. Rev. B, 77, 245117, 2008.
3. Eilmes A., Petelenz P., Model calculations of local exciton levels in the C_{60} fullerene crystals doped with endohedral fullerides $M@C_{60}$, Chem.Phys., 237, 67–72, 1998.
4. Eilmes A., Petelenz P., Effects of microscopic disorder in electroabsorption spectroscopy: Orientational disorder in the fullerene crystal, J. Chem. Phys., 118, 3711–3716, 2003.
5. Eilmes A., Pac B., Petelenz P., Temperature dependence of the spectral profile and total intensity of the second-harmonic signal of the fullerene crystal, J. Chem. Phys., 130, 074701, 2009.
6. Eilmes A., Munn R.W., Microscopic calculation of the energetics of charged states in amorphous polyethylene, J. Chem. Phys., 120, 7779–7783, 2004.
7. Scarle S., Sterzel M., Eilmes A., Munn R.W., Monte Carlo simulations of Li^+ motion in polyethylene based on polarization energy calculations and informed by data compression analysis, J. Chem. Phys., 123, 154909, 2005.
8. Eilmes A., Kubisiak P., Quantum-chemical study on the effect of Lewis acid centers in poly(ethylene oxide)-based solid electrolyte, J. Phys Chem. A, 111, 6388–6396, 2007.
9. Eilmes A., Kubisiak P., Polarizable Continuum Model study on the solvent effect of polymer matrix in poly(ethylene oxide)-based solid electrolyte, J. Phys. Chem. A, 112, 8849–8857, 2008.

Julita Eilmes

Dr habil, PhD

Research profile

Organic synthesis; Supramolecular chemistry; Dibenzotetraaza[14]annulenes; Schiff bases; DNA/RNA binding agents; Liquid crystals

Associate Professor in Organic Chemistry Department and Head of Supramolecular and Biomimetic Chemistry Group. She has supervised seven PhD and twenty MSc theses. Currently she teaches Supramolecular Chemistry, Chemistry of Macrocyclic Complexes and Recent Advances in Organic Synthesis to MSc chemistry students further to supervising Advanced Organic Synthesis Laboratory.

Current members of the research group: Łukasz Dudek, PhD, Jarosław Grolik, PhD, Krzysztof Zwoliński, MSc.

Research areas: The research interests of the group revolve around the problems of the synthesis and supramolecular chemistry of macrocyclic ligands and of Schiff bases and their complexes with transition metals. The present group activity is aiming at preparation of new liquid crystalline materials, as well as of novel dibenzotetraaza[14]annulene derivatives of potential biomedical importance.

Ongoing research projects: (i) New dicationic derivatives of dibenzotetraaza[14]annulene: tuning DNA/RNA binding properties; (ii) Design and synthesis of mesogens, metallomesogens and lacunar-type receptors based on dibenzotetraaza-[14]annulene; (iii) New macrocyclic receptors of anions and neutral molecules.

Selected publications

1. Pawlica D., Radić-Stojković M., Sieroń L, Piantanida I., Eilmes J., Synthesis, crystal structures and the preliminary evaluation of the new dibenzotetraaza[14]annulene-based DNA/RNA binding agents, Tetrahedron 62, 9156–9165, 2006.
2. Grolik J., Sieroń L., Eilmes J., New liquid crystalline derivative of dibenzotetraaza[14]-annulene: synthesis, characterization and the preliminary evaluation of mesomorphic properties, Tetrahedron Lett., 47, 8209–8213, 2006.
3. Radić-Stojković M., Piantanida I., Kralj M., Marjanowic M., Zinic M., Pawlica D., Eilmes J., The dicationic derivatives of DBTAA: Interactions with DNA/RNA and antiproliferative effects on human cell lines, Bioorg. Med. Chem., 15, 1795–1801, 2007.
4. Grolik J., Dominiak P. M., Sieroń L., Woźniak K., Eilmes J., New lacunar type and pendant groups containing derivatives of β-unsubstituted dibenzotetraaza[14]annulenes – syntheses and crystal structures, Tetrahedron, 64, 7796–7806, 2008.
5. Pawlica D., Radić-Stojković M., Sieroń L, Dudek Ł., Piantanida I., Eilmes J., New dicationic derivatives of dibenzotetraaza[14]annulene: tuning DNA binding properties, Tetrahedron, 65, 3980–3989, 2009.

Marek Frankowicz

Dr habil, PhD

Research profile

Theoretical chemistry; Nonlinear chemical dynamics; Stochastic simulations; Theory of complexity

Post-Doctoral Fellow at Free University of Brussels (1981–82) and Tokyo University (1982–83); Lecturer at University Paris 6 (1988–90); Member of the Advisory Board of the international journal "Interdisciplinary Description of Complex Systems" (INDECS).

Current research interests: Stochastic dynamics of nonlinear chemical systems, foundations of thermodynamics, applications of complexity theory (complex adaptive systems, active walks in adaptive landscapes) to natural and social systems; Operations research; Modelling of dynamics of higher education reforms in Europe.

Selected publications

1. Frankowicz M., Nicolis G., Transient evolution towards a unique stable state: stochastic analysis of explosive behavior in a chemical system, J. Stat. Phys., 33, 595–609, 1983.
2. Frankowicz M., Malek-Mansour M., Nicolis G., Stochastic analysis of explosive behavior: a qualitative approach, Physica A, 125, 237–246, 1984.
3. Frankowicz M., Kawczynski A.L., Stochastic effects in front propagation: the acetylcholinesterase reaction, J. Phys. Chem., 93, 2755–2759, 1989.
4. Shiino M., Frankowicz M., Synchronization of infinitely many coupled limit-cycle type oscillators, Phys. Lett. A, 136, 103–108, 1989.
5. Frankowicz M., Kawczynski A.L., Gorecki J., Stochastic effects in propagation of impulses: the Belousov-Zhabotinskii reaction, J. Phys. Chem., 95, 1265–1268, 1991.
6. Martinas K., Frankowicz M., Extropy – reformulation of the entropy principle, Period. Polytech. Chem., 44, 29–38, 2000.
7. Jagoda-Ćwiklik B., Ćwiklik L., Frankowicz M., Simulations of temperature programmed desorption spectra from porous surface, Appl. Surf. Sci. 219, 276–281, 2003.
8. Frankowicz M., Chrenowski M., Application of Preisach model to adsorption desorption hysteresis, Physica B, 372, 219–221, 2006.
9. Frankowicz M., Il Processo di Bologna in Pologna, in: IX Profilo dei laureati italiani. La riforma allo specchio, Il Mulino, Bologna 2007, pp. 409–413.

Stanisław Andrzej Hodorowicz

Professor of Chemistry, Dr habil, PhD

Research profile

Solid State Chemistry; Crystallography

Born 9 March 1941, Bukowina Tatrzańska, Poland; Education: MSc, 1970, PhD 1974, Habilitation (Solid State Chemistry), 1979, Jagiellonian University; Postdoctoral studies in crystallography, Leningrad State University 1978, and in inorganic chemistry, Michigan University, USA, 1981–83.

Appointments: Head of the Department of Crystal Chemistry and Crystal Physics, 1979–1981, 1984–90; Deputy Head of the Institute of Chemistry, 1980–81; Dean of the Faculty of Chemistry, 1981–86, 1987–93; Vice-Rector of the Jagiellonian University, 1993–2000; Rector of the Podhalańska State Higher Education Vocational School, Nowy Targ, 2001–present.

Memberships: IUPAC International Committee; The Board of the Polish Chemical Society (former); Vice-President of the Committee of Crystallography of the Polish Academy of Sciences; President of the Polish Crystal Growth Society (former); President of the Foundation of the Jagiellonian University (former); President of the Polish Crystallographic Association.

Selected publications

1. Barszcz B., Hodorowicz S.A., Stadnicka K., Jabłońska-Wawrzycka A., A comparision of the coordination geometries of some 4-methylimidozolo-5carbaldehyde complexes with Zn(II), Cd(II) and Co(II) loss in the solid state and aqueous solution, Polyhedron, 24, 627–637, 2005.
2. Barszcz B., Jabłońska-Wawrzycka A., Stadnicka K., Hodorowicz S.A., The synthesis and structural characterization of novel zinc and cadmium complexes of chelating alcohol, Inorg. Chem. Commun., 8, 951–954, 2005.
3. Michalec M., Stadnicka K., Hodorowicz S.A., Crystal structure of pyridinium isopolymolybdate $(C_5H_6N)_{2n}[Mo_4O_{13}]_n$, Cryst. Res. Technol., 42, 91–97, 2006.
4. Kotarba A., Barański A., Hodorowicz S., Sokołowski J., Szytuła A., Holmlid L., Stability and excitation of potassium promoter in iron catalysts – the role of $KFeO_2$ and $KAlO_2$ phases, Catal. Lett., 67, 129–134, 2000.

Janusz Jamrozik

Dr habil, PhD

Research profile

Organic chemistry; Polycyclic compounds; Propellanes; Spiranes

PhD, 1969; Habilitation, 1985; Research Fellow at Universities of Goettingen, 1983, and Wyoming, Laramie, USA, 1986–87; Visiting Professor at the University of Heidelberg, 1993–1995 (short term stays); Vice-Dean of the Faculty of Chemistry, 1987–1991, 1999–2005; Head of the Organic Chemistry Department, 1994–2000.

Research interests: Propellanes are the group of tricyclic compounds in which one bond is common for three rings. The structure of propellane is similar to propeller and it occurs also in natural compounds. My investigations concern especially synthesis and structural studies of polypropellane and polyspiran compounds. I explained why a starting material that may apparently give a propellane or a dispiran, sometimes gives only one of these products. The formation of propellanes or of the isomeric dispirans depends on the nature of the heteroatom. Some aspects of the conformation of the compounds were studied. Energy calculations were carried out to find the preferred conformations. In my laboratory a new method of synthesis of bispropellanes from tetramethyl derivatives of biphenyl or benzene was invented. Alongside I am investigating bridge[4.3.3]propellanes and another group of propellanes which derives from 1,6-methano[10]annulene.

Selected publications

1. Jamrozik J., Żak G., Grochowski J., Markiewicz M., Serda P., The structure of substituted spirans derived from benzo-1,5-dithiepine and benzo-1,5-dioxepine systems. Ring-reversal isomers, J. Mol. Struct., 687, 79–86, 2004.
2. Jamrozik J., Żak G., Grochowski J., Markiewicz M., Serda P., Structural characterization of new dispiranes and postulated molecular structure of their propellane isomers, J. Mol. Struct., 691, 39–44, 2004.
3. Jamrozik J., Szlachcic P., Synthesis of trioxa[8.3.1] and [13.3.1]propellanes from 1,1,2,2-tetrakis(bromomethyl)cyclopropane, Polish. J. Chem., 74, 1363–1367, 2000.
4. Barańska J., Grochowski J., Jamrozik J., Serda P., New spirant containing a 1,5-benzodithiepine system, derived from methylbenzenes. Conformational transmission, Org. Lett., 2, 425–427, 2000.
5. Jamrozik J., Szlachcic P., Synthesis of substituted 8,11-dioxa(3,4-benzo)-[4.3.3]propellanes, Polish. J. Chem., 75, 1881–1885, 2001.
6. Jamrozik J., Żesławski W., Bis- und tris(propellane) aus methylbenzolen: 1,2;3,4;5,6-tris{8',11'-dioxa[4.3.3]propella(3',4')}benzol, Chem. Ber., 127, 2471–2473, 1994.
7. Jaeger D.A., Węgrzyn-Clennan M., Jamrozik J., Monohalogenation of alkyl phenyl ethers in micellar and vesicular media, J. Am. Chem. Soc., 112, 1171–1176, 1990.

Marian Jaskuła

Dr habil, PhD

Research profile

Physical chemistry; Electrochemistry; Metal deposition and dissolution; Industrial electrolysis; Nanotechnology; Self-organizing nanostructures; Fuel cells; Lithium-ion batteries

Ausserplanmässiger Professor, Technical University, Aachen Germany; Honorary Professor at the Kiev National University of Technology & Design, Ukraine; Head of the Electrochemistry Group at the Jagiellonian University.

Research associates: Grzegorz Sulka, PhD, Tadeusz Bieszczad, PhD, Joanna Kapusta, MSc, Agnieszka Brzózka, MSc, Leszek Zaraska, MSc.

The interest of our group concentrates on various aspects of basic and industrial electrochemistry, new materials and nanotechnology, especially on the field of non-ferrous and noble metals, and includes the following topics:

- deposition and dissolution of metals and alloys,
- copper electrorefining process at high current densities,
- behavior of silver during copper electrorefining,
- mechanism and kinetics of silver ion cementation on metallic copper,
- metal-matrix composites and their properties,
- anodisation of aluminum and self organizing structures,
- new electrode materials for electrochemical cells,
- practical applications of ion-selective electrodes.

Selected publications

1. Lykhnytskyi K.V., Barsukov V.Z., Jaskuła M., Promising catalysts for H_2-O_2 fuel cells (Review) in: Hydrogen Materials Science and Chemistry of Carbon Nanomaterials, Najat Veziroglu T. (Ed.), Springer 2007, pp.177–185.
2. Sulka G.D., Highly ordered anodic porous alumina formation by self-organised anodising and template-assisted fabrication of nanostructured materials, in: Nanostructured Materials in Electrochemistry, Eftekhari A. (Ed.), Wiley-VCH 2008, pp. 1–116.
3. Bech-Nielsen G., Jaskuła M., The Influence of a magnetic field on the non-electrochemical dissolution of iron, J. Electroanal. Chem., 624, 327–328, 2008.
4. Medelienė V., Juđkėnas R., Kurtinaitienė M., Jaskuła M., Copper metal matrix composite Cu-TiO_2 electrodeposited in aqueous suspensions of the nanometric size particles of anatase and rutile, Polish J. Chem., 78, 1305–1317, 2004.
5. Barsukov V., Il'yn E., Jaskuła M., New active materials for negative electrodes of lithium-ion batteries, Electrochem. Power Eng., 2, 153–164, 2002.
6. Sulka G.D., Jaskuła M., Effect of sulphuric acid and copper sulphate concentrations on the morphology of silver deposit in the cementation process, Electrochim. Acta, 51, 6111–6119, 2006.

Adam Juszkiewicz

Professor of Chemistry, Dr habil, PhD

Research profile

Environmental chemistry; Environmental chemical analysis

Head of the Department of General Chemistry from 1996 to present; Organizer and the first Director of the Course of Studies in Environmental Protection at the Jagiellonian University; Member of the Committee for Environmental Impact Assessment at the Ministry of Environment (1994–2003); Member of the State Council for Environmental Protection (2003–2007); Specialist in physical chemistry of solutions and in environmental chemistry.

Current research projects:

1. Determination of organic and inorganic toxicants in soil, water and air using chromatographic and spectrophotometric methods.
2. Determination of organic compounds released from insulation building materials.

Selected publications

1. Juszkiewicz A., Kijak B., Traffic generated air pollution with volatile organic compounds in Kraków and its environs, Polish J. Environ. Stud., 12, 49–56, 2003.
2. Byrski W., Juszkiewicz A., Identification of characteristic of ultrasonic sensor used for density measurements in chemical process aimed at control education, Proceedings of the 7th World Multiconference of Systemics, Cybernetics and Informatics, Orlando, Florida (USA), 2003, vol. 1, 125–130.
3. Juszkiewicz A., Zaborska W., Sepioł J., Góra M., Zaborska A., Inactivation of jack bean urease by allicin, J. Enzym. Inhib. Med. Chem., 18, 419–424, 2003.
4. Choczyński M., Nęcki J.M., Juszkiewicz A., Determination of rate constants and activation energies for emission of organic compounds from polyoxymethylene, Acta Chromatogr., 14, 37–48, 2004.
5. Juszkiewicz A., Zaborska A., Łaptaś A., Olech Z., A study of the inhibition of jack bean urease by garlic extract, Food Chemistry, 85, 553–558, 2004.
6. Juszkiewicz A., Kijak B., Lotne węglowodory w powietrzu atmosferycznym. Czym oddychamy w Krakowie? Aura, 3, 8–10, 2006.
7. Juszkiewicz A., Bartynowska-Meus Z., Kawałek M., Meus M., Łaptaś A., Wpływ oczyszczalni ścieków na jakość wód dorzecza Rudawy, Aura, 6, 12–14, 2006.
8. Zaborska W., Karcz W., Kot M., Juszkiewicz A., Modification of jack bean urease thiols by tiosulfinates contained in garlic extract. DTNB titration studies, Food Chem., 112, 42–45, 2009.

Jacek Korchowiec

Dr habil, PhD

Research profile

Quantum and computational chemistry; Conceptual density functional theory; Linear scaling methods; Theory of chemical reactivity

My research is concerned with theory of chemical reactivity and development of linear scaling methods. Among my achievements are: charge sensitivity analysis (CSA), self-consistent charge and configuration method for subsystems (SCCCMS), regional localized molecular orbitals (RLMO), elongation (ELG) and elongation cutoff (ELG/C) methods.

The CSA is a formalism rooted in density functional theory allowing studies of system responses to hypothetical perturbations. The method was formulated in different resolutions starting from local to global one, via intermediate molecular orbital, atoms-in-molecule and fragment resolutions. The concepts derived within CSA were used by SCCCMS for partitioning the system interaction energy into physically justified components. ELG and ELG/C methods by contrast, belong to the family of fragmentation techniques which were developed for computing the electronic structure of huge molecular systems. The ELG and ELG/C methods are formulated at Hartree-Fock and Kohn-Sham levels of theory for both closed- and open-shell systems. The ELG/C scheme takes the full advantage of RLMO basis and can be considered as a very efficient sparse matrix algebra scheme.

Selected publications

1. Korchowiec J., Lewandowski J., Makowski M., Gu F.L., Aoki Y., Elongation cutoff technique armed with quantum fast multipole method for linear scaling, J. Comput. Chem., 2009, in press.
2. Korchowiec J., Korchowiec B., Priebe W., Rogalska E., DFT study on the selectivity of complexation of metal cations with a dioxadithia crown ether ligand, J. Phys. Chem A., 112, 13633–13640, 2008.
3. Gu F.L., Aoki Y., Korchowiec J., Imamura A., Kirtman B., A new localization scheme for the elongation method, J. Chem. Phys., 121, 10385–10391, 2004.
4. Korchowiec J., Uchimaru T., New energy partitioning scheme based on the self-consistent charge and configuration method for subsystems: Application to water dimer system, J. Chem. Phys., 112, 1623–1633, 2000.
5. Nalewajski R.F., Korchowiec J., Charge Sensitivity Approach to Electronic Structure and Chemical Reactivity, Advances Series in Physical Chemistry, Vol 8, World Scientific, Singapore, 1997.

Paweł Kościelniak

Professor of Chemistry, Dr habil, PhD

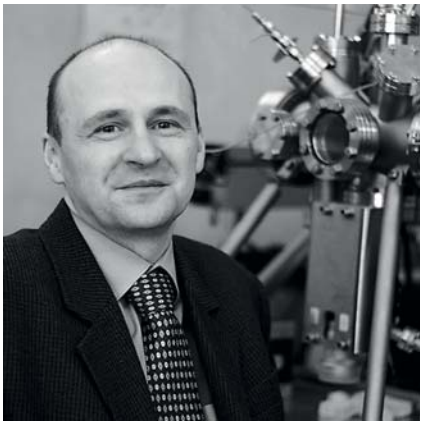
Research profile

Analytical chemistry; Flow analysis; Forensic chemistry

I am Head of the *Analytical Flow Techniques* research group at the Department of Analytical Chemistry. We are involved in the development of new analytical methods and procedures in flow analysis and forensic chemistry with special attention paid to such fundamental analytical issues as calibration, interference effects, digestion, preconcentration and separation. Our scientific interest is also in the design of original flow devices dedicated to defined analytical purposes. For instance, we are the authors of a versatile flow injection manifold allowing different calibration methods to be realized in simple, fast and cost-effective manner. In addition, we are focused on miniaturization of flow systems and their adaptation to clinical and forensic analysis (e.g. to detection and determination of psychotropic drugs in saliva). Also, in collaboration with the Institute of Forensic Research, Kraków, we develop novel analytical approaches to identification and comparison of various forensic traces (e.g. inks, paints, explosives). Our laboratories are equipped with modern analytical instruments, including ICP-OES, ICP-MS, AAS, AFS, HPLC, GC and capillary electrophoresis systems. Apart from the above research we offer attractive study courses giving students a chance to exploit analytical knowledge and skills in environmental, toxicological, pharmaceutical, clinical and forensic areas.

Selected publications

1. Kościelniak P., Wieczorek M., Kozak J., Herman M., Versatile flow injection manifold for analytical calibration, Anal. Chim. Acta, 600, 6–13, 2007.
2. Woźniakiewicz M., Wietecha-Posłuszny R., Garbacik A., Kościelniak P., Microwave-assisted extraction of tricyclic antidepressants from human serum followed by high performance liquid chromatography determination, J. Chromatogr. A, 1190, 52–56, 2008.
3. Zięba-Palus J., Zadora G., Milczarek J.M., Kościelniak P., Pyrolysis-gas chromatography/mass spectrometry analysis as a useful tool in forensic examination of automotive paint traces, J. Chromatogr. A, 1179, 41–46, 2008.
4. Madej K., Kościelniak P., Review of analytical methods for identification and determination of phenothiazines and tricyclic antidepressants, Crit. Rev. Anal. Chem., 38, 51–67, 2008.
5. Kozak J., Wójtowicz M., Wróbel A., Kościelniak P., Novel approach to calibration by the complementary dilution method with the use of a monosegmented sequential injection system, Talanta, 77, 587–592, 2008.
6. Wójtowicz M., Kozak J., Górnacka D., Kościelniak P., Application of flow injection gradient titration based on a sample and standard dilution to the determination of total acidity in vinegars and soft drinks, Anal. Sci., 24, 1593–1597, 2008.
7. Kościelniak P., Advanced calibration methods in flow injection analysis, in: Advances in Flow Analysis, Trojanowicz M. (Ed.), Wiley-VCh,, Weinheim 2008, pp. 203-226.



Andrzej Kotarba

Dr habil, PhD

Research profile

Solid state and surface chemistry; Inorganic nanomaterials; Catalysts; Metal implants

Appointments: Study Programmes Coordinator for the Inter-Faculty Course of Studies in Advanced Materials and Nanotechnology; Head of the Materials and Surface Chemistry group.

The main goal of research in our group is to gain an understanding of the processes taking place at the solid/gas interfaces to further apply it in designing the surfaces with desired properties. We conduct research on the preparation of new solid materials, modification of their surfaces, and characterization of their reactivities (adsorption/desorption of reactants, catalytic screening). The motivation for the research is both fundamental (interaction of small molecules with model surfaces, modification of surface electronic properties by alkali doping) and practical (characterization of real catalysts; expert works for chemical companies Norsk Hydro, INS Puławy, Süd Chemie; patents on new catalytic materials; engineering of metal implant surfaces).

More information: www.chemia.uj.edu.pl/kotarba

Selected publications

1. Kotarba A., Kruk I., Sojka Z., Energetics of potassium loss from styrene catalyst model components – Reassignment of K-storage and release phases, J. Catal., 211, 265–272, 2002.
2. Kotarba A., Dmytrzyk J., Raróg-Pilecka W., Kowalczyk Z., Surface heterogeneity of Cs promoter in carbon-based ruthenium catalyst for ammonia synthesis, Appl. Surf. Sci., 207, 327–333, 2003.
3. Kotarba A., Adamski G., Piskorz W., Sojka Z., Sayag C., Djega-Mariadassou G., Manipulation of Fermi level in Mo_2C catalyst by potassium doping: Impact on the reactivity in HDN of indole, J. Phys. Chem. B, 108, 2885–2892, 2004.
4. Kotarba A., Rożek W., Serafin I., Sojka Z., Reverse effect of doping on stability of principal components of styrene catalyst: $KFeO_2$ and $K_2Fe_{22}O_{34}$, J. Catal., 247, 238–244, 2007.
5. Stelmachowski P., Maniak G., Kotarba A., Sojka Z., Strong electronic promotion of Co_3O_4 towards N_2O decomposition by surface alkali dopants, Catal. Commun., 10, 1062–1065, 2009.
6. Cieślik M., Reczyński W., Janus A.M., Engvall K., Socha R.P., Kotarba A., Metal release and formation of surface precipitate at stainless steel grade 316 and Hanks solution interface – Inflammatory response and surface finishing effects, Corros. Sci., 2009, doi:10.1016/j.corsci.2009.02.012.
7. Kotarba A., Holmlid L., Energy-pooling transitions to doubly excited K atoms at a promoted iron-oxide catalyst surface: more than 30 eV available for reaction, Phys. Chem. Chem. Phys., 2009, doi:10.1039/B817380J.

Barbara Krajewska

Dr habil, PhD

Research profile

(Bio)polymers (chitosan) as biomedical materials; Enzymes (urease) free and immobilized; Membrane separation processes; Biocatalysis

My scientific interest is in (bio)polymeric functional materials and their bio-applications. These include areas such as biomedical materials, separation processes, biosensors, and importantly, immobilization of enzymes. The utilization of enzymes is special in that it is one of chief present strategies towards environmentally benign and energy- and material-saving chemical processes. The polymer and enzyme I concentrate on are chitosan and urease. Chitosan, a polyaminosaccharide from renewable resources offers a unique beneficial set of bio-characteristics. Urease by contrast, is an enzyme of crucial importance in medical, analytical and novel engineering areas. I study chitosan as a biomaterial and as a urease immobilization support, also urease in its native and chitosan-immobilized form, and interfacial phonemena taking place in the chitosan-urease system.

Selected publications

1. Krajewska B., Ureases. I. Functional, kinetic and catalytic properties: a review, J. Mol. Catal. B: Enzym., 59: 9–21, 2009.
2. Krajewska B., Ureases. II. Properties and their customizing by enzyme immobilizations: a review, J. Mol. Catal. B: Enzym., 59: 22–40, 2009.
3. Alatorre-Meda M., Taboada P., Sabin J., Krajewska B., Varela L.M., Rodriguez J.R., DNA-chitosan complexation: A dynamic light scattering study, Colloid. Surface. A, 339, 145–152, 2009.
4. Krajewska B., Mono- (Ag, Hg) and di- (Cu, Hg) valent metal ions effects on the activity of jack bean urease. Probing the modes of metal binding to the enzyme, J. Enzym. Inhib. Med. Chem., 23, 535–542, 2008.
5. Wydro P., Krajewska B., Hąc-Wydro K., Chitosan as a lipid binder. A Langmuir monolayer study of chitosan-lipid interactions, Biomacromolecules, 8, 2611–2617, 2007.
6. Ehrlich H., Krajewska B., Hanke T., Born R., Heinemann S., Knieb C., Worch H., Chitosan membrane as a template for hydroxyapatite crystal growth in a model dual membrane diffusion system, J. Membrane Sci., 273, 124–128, 2006.
7. Krajewska B., Ciurli S., Jack bean (*Canavalia ensiformis*) urease. Probing acid-base groups of the active site by pH-variation, Plant Physiol. Biochem., 43, 651–658, 2005.
8. Krajewska B., Piwowarska Z., Free vs chitosan-immobilized urease. Microenvironmental effects on enzyme inhibitions, Biocatal. Biotransfor., 23, 225–232, 2005.
9. Krajewska B., Membrane-based processes performed with use of chitin/chitosan materials, Sep. Purif. Technol., 41, 305–312, 2005.
10. Krajewska B., Application of chitin- and chitosan-based materials for enzyme immobilizations: a review, Enzyme Microb. Tech., 35, 126–139, 2004.
11. Krajewska B., Diffusion of metal ions through gel chitosan membranes, React. Funct. Polym., 47, 37–47, 2001.

Krzysztof Kruczała

Dr habil, PhD

Research profile

Fuel cell; Polymer degradation and stabilization; Spectroscopy; EPR/ESR

My studies are related to processes of degradation and stabilization in ionic polymers and thermoplastics. One of the main aims of this type of research is to determine the lifetime of polymeric materials by finding and understanding the relationships between structure, morphology and amount of additives. The research includes commercial polymers such as ABS, NAFION, PAA and others which are widely used in automotive industry as well as in fuel cells with polymer electrolyte membranes. The main goal of current research is to determine the influence of transition metal ions on the stability of membrane electrolyte assembly used in PEM FC. The research is performed in collaboration with University of Detroit Mercy, USA. The results of my research were published in ISI journals (22 articles), in peer-reviewed conference proceedings (5 publications) and were presented at 43 conferences. I co-authored three chapters in the English-language books relating to the application of electron paramagnetic resonance spectroscopy and EPR imaging in the study of polymers. I have been twice honoured with the Team Award of the Rector of the Jagiellonian University.

Contact information: phone (+12) 6632224; e-mail: kruczala@chemia.uj.edu.pl

Selected publications

1. Kruczała K., Motyakin M., Schlick S., J. Phys. Chem. B, 104, 3387–3392, 2000.
2. Podgajny R., Dromzee Y., Kruczała K., Sieklucka B., Polyhedron, 20, 685–694, 2001.
3. Kruczała K., Varghese B., Bokria J.G., Schlick S., Macromolecules., 36, 1899–1908, 2003.
4. Kruczała K., Bokria J.G., Schlick S., Macromolecules, 36, 1909–1919, 2003.
5. Podgajny R., Korzeniak T., Stadnicka K., Drodze Y., Alcock N.W., Errington W., Kruczała K., Balanga M., Kemp T.J., Verdaguer M., Sieklucka B., Dalton T., 17, 3458–3468, 2003.
6. Kruczała K., Aris W., Schlick S., Macromololecules., 38, 6979–6987, 2005.
7. Spalek T., Kruczała K., Sojka Z., Schlick S., J. Magn. Reson., 189, 139–150, 2007.
8. Kruczała K., Szczubiałka K., Łańcucki Ł, Zastawny I., Góra-Marek K., Dyrek K., Sojka Z., Spectrochim. Acta A, 69, 1337–1343, 2008.
9. Gustafsson H., Kruczała K., Lund E., Schlick S., J. Phys. Chem. B, 112, 8437–8442, 2008.
10. Kozieł M., Podgajny R., Kania R., Lebris R., Mathoniere C., Lewinski K., Kruczała K., Rams M., Labrugere C., Bousseksou A., Sieklucka B., Inorg. Chem., 49, 2765–2772, 2010.
11. Schlick S., Kruczała K., Spatially-resolved degradation in heterophasic polymers from 1D and 2D spectral-spatial ESR imaging experiments, in: Advanced ESR Methods in Polymer Research, Schlick S. (Ed.), Wiley, 2006, Chapter 10, pp. 229–254.

Piotr Kuśtrowski

Dr habil, PhD

Research profile

Heterogeneous catalysis; Oxide-type catalysts for transformation of hydrocarbons; Adsorption of air and water pollutants; Cationic and anionic clays; Mesoporous sieves

Habilitation, 2007, Jagiellonian University
PhD, 2000, Jagiellonian University
MSc, 1995, Jagiellonian University

Head of Organic Technology research group (since 2008).
Main research topics: Synthesis of novel hydrotalcite-like layered materials modified with transition metal cations (e.g. Cu^{2+}, Ni^{2+}, Fe^{3+}, Cr^{3+}) and various interlayer anions (e.g. dicarboxylic anions, polyoxoanions); Application of molecular designed dispersion method for modification of mesoporous molecular sieves (e.g. MCM-48, SBA-15, MCF, MSU-x) with transition metal oxides; Development of new catalytic processes for olefin production – oxidative dehydrogenation of saturated hydrocarbons with carbon dioxide and nitrous oxide; Activation of natural and synthetic inorganic materials for the N_2O decomposition; Investigation of acidic and basic properties of inorganic materials by test reactions (e.g. MBOH conversion, aldol condensation, cumene cracking, isopropanol conversion); Development of new types of adsorbents and catalysts for removal of air and water pollutants by selective adsorption and total oxidation processes; Synthesis of high surface area silicas and aluminosilicas using polymer matrices based on swelling cross-linked gels.

Selected publications

1. Kuśtrowski P., Chmielarz L., Dziembaj R., Cool P., Vansant E.F., Dehydrogenation of ethylbenzene with nitrous oxide in the presence of mesoporous silica materials modified with transition metal oxides, J. Phys. Chem. A, 109, 330–336, 2005.
2. Segura Y., Chmielarz L., Kuśtrowski P., Cool P., Dziembaj R., Vansant E.F., Preparation and characterization of vanadium oxide deposited on thermally stable mesoporous titania, J. Phys. Chem. B, 110, 948–955, 2006.
3. Serafin I., Kotarba A., Grzywa M., Sojka Z., Bińczycka H., Kuśtrowski P., Quenching of potassium loss for styrene catalyst: Effect of Cr doping on stabilization of the $K_2Fe_{22}O_{34}$ active phase, J. Catal., 239, 137–144, 2006.
4. Kuśtrowski P., Sułkowska D., Chmielarz L., Dziembaj R., Aldol condensation of citral and acetone over mesoporous catalysts obtained by thermal and chemical activation of magnesium-aluminum hydrotalcite-like precursors, Appl. Catal. A, 302, 317–324, 2006.
5. Michorczyk P., Ogonowski J., Kuśtrowski P., Chmielarz L., Chromium oxide supported on MCM-41 as a highly active and selective catalyst for dehydrogenation of propane with CO_2, Appl. Catal. A, 349, 62–69, 2008.

Krzysztof Lewiński

Dr habil, PhD

Research profile

Crystal structure; Proteins; High-pressure protein crystallography; Enzymes

Research interest is focused on structural investigations using single crystal X-ray diffraction methods. Among recent projects are:

- determination of high-pressure crystal structure of selected proteins (ribonuclease A, insulin, BPTI, hemoglobin, thaumatin),
- structural origin of decreased pressure and temperature stability of mutated ribonuclease A molecules,
- crystal structure of human arylsulfatase A, its enzymatic mechanism and inhibition,
- specificity of ligand binding by beta-lactoglobuline,
- synthesis and structural investigations of new organic compounds with potential biological activity,
- structural investigations of mixed-ligand cyanocomplexes of molybdenum and of supramolecular assemblies based on octacyanotungstate(V).

Selected publications

1. Chagnault V., Compain P., Lewinski K., Ikeda K., Asano N., Martin O.R., Stereodivergent access to polyhydroxylated 10-azabicyclo[4.3.1]decanes as new calystegine analogs, J. Org. Chem., 74, 3179–3182, 2009.
2. Matoga D., Szklarzewicz J., Lewiński K., Cyanooxo molybdenum(IV) complexes with 2-pyrazinecarbonitrile and 2-pyrazinecarboxylate: Crystallographic and spectroscopic studies reveal metal-assisted nitrile hydrolysis, Polyhedron, 27, 2643–2649, 2008.
3. Przychodzeń P., Pełka R., Lewiński K., Supel J., Rams M., Tomala K., Sieklucka B., Tuning of magnetic properties of polynuclear lanthanide(III)-octacyanotungstate(V) systems: Determination of ligand-field parameters and exchange interaction, Inorg. Chem., 46, 8924–8938, 2007.
4. Ciechanowicz-Rutkowska M., Lewiński K., Oleksyn B., Stec B., Model studies of the function of blockers on the small conductance potassium ion channel, J. Pept. Res., 62, 1–9, 2003.
5. Chruszcz M., Laidler P., Monkiewicz M., Ortlund E., Lebioda L., Lewiński K., Crystal structure of a covalent intermediate of endogenous human arylsulfatase A, J. Inorg. Biochem., 96, 386–392, 2003.
6. Ortlund E., LaCount M.W., Lewiński K., Lebioda L., Reactions of *Pseudomonas* 7A glutaminase-asparaginase with diazo analogs of glutamine and asparagine result in unexpected covalent inhibitions and suggests an unusual catalytic triad Thr-Tyr-Glu, Biochemistry, 39, 1199–1204, 2000.
7. Jakob C.G., Lewiński K., Kuciel R., Ostrowski W., Lebioda L., Crystal structure of prostatic acid phosphatase, Prostate, 42, 211–218, 2000.

Maria Łabanowska

Dr habil, PhD

Research profile

ESR of transitions metals ions in heterogeneous catalysts and biological systems; Radical processes in biological systems

Maria Łabanowska was born in Kraków. She completed her PhD at the Jagiellonian University and in 2003 she qualified as an associate professor. Her professional experience includes research posts at the Medical University of Kraków, Institute of Petrotechnology and Regional Laboratory of Physicochemical Analyses and Structural Research, as well as academic visits to the Universities of Bologna and Pierre and Marie Curie in Paris. Her research interests include processes occurring at the gas/solid interface and chemistry of transition metal ions in relation to heterogeneous catalysts and to biological materials investigated mainly by ESR technique. In 2003 she began research on physicochemical properties of starch, mainly those resulting from radical processes occurring upon physical, chemical and enzymatic modifications. Recently she has broadened her scientific interest to raw biological systems. Within the Department of Inorganic Chemistry, she is Head of the Cryogenics and Food Chemistry group.

Selected publications

1. Łabanowska M., Paramagnetic defects in MoO_3 – Revisited, Phys. Chem. Chem. Phys., 1, 5385–5392, 1999.
2. Dyrek K., Łabanowska M., Rembertowicz H., Bidzińska E., Electron paramagnetic resonance study of V_2O_5 deactivation in the course of catalytic oxidation of SO_2 to SO_3, Spectrochim. Acta A, 56, 309–318, 2000.
3. Łabanowska M., Electron paramagnetic resonance study of interaction between MoO_3 and propene, Phys. Chem. Chem. Phys., 2, 3307–3311, 2000.
4. Łabanowska M., EPR monitoring of redox processes in transition metal oxide catalyst, Chem. Phys. Chem., 2, 712–731, 2001.
5. Bastardo-Gonzales E., Jones W., Bahranowski K., Łabanowska M., Serwicka E.M., ESR Investigations of vanadium centres supported on Al-containing mesoporous silica, Micropor. Mesopor. Mat., 50, 61–72, 2001.
6. Bidzińska E., Dyrek K., Fortuna T., Łabanowska M., Pietrzyk S., EPR studies of the thermally treated oxidized corn starch, Starch/Stärke, 56, 461–468, 2004.
7. Łabanowska M., Bidzińska E., Dyrek K., Szymońska J., Electron paramagnetic resonance study of water distribution in starch granules, Biopolymers, 82, 549– 557, 2006.
8. Dyrek K., Bidzińska E., Łabanowska M., Fortuna T., Przetaczek I., Pietrzyk S., EPR study of radicals generated in starch by microwaves or by conventional heating, Starch/Stärke, 59, 318–325, 2007.
9. Łabanowska M., Bidzińska E., Dyrek K.,.Fortuna T., Pietrzyk S., Rożnowski J., Socha R.P., Cu^{2+} ions as a paramagnetic probe in EPR studies of radicals generated thermally in starch, Starch/Stärke, 60, 134–145, 2008.

Wiesław Łasocha

Professor of Chemistry, Dr habil, PhD

Research profile

Powder diffractometry; Synthesis of new materials

Areas of research and techniques used:

1. Structural studies of materials using powder diffraction data; Optimisation and testing of new methods of structural powder diffraction.

2. Inorganic synthesis and structural investigations of new fibrillar and layered hybrid inorganic-organic materials, new isopolycompounds of aliphatic and aromatic amines, and of new peroxomolybdates, peroxovanadates and peroxotungstates.

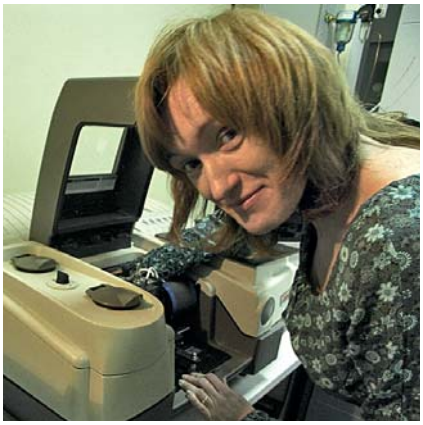
3. Investigations of the objects of cultural heritage by X-ray methods.

Experience and achievements:
I have worked in laboratories in the USA and the Netherlands co-operating with Professors Harry Eick and Henk Schenk (past president of the International Union of Crystallography). Since 1997 my group has closely co-operated with the International Centre for Diffraction Data (USA) on powder diffraction characterisation of new materials. I have authored and co-authored over 100 scientific papers. Since 2005 I am also Head of the Laboratory of X-ray Diffraction in the Institute of Catalysis of the PAS.

More information: http://www.chemia.uj.edu.pl/~lasocha

Selected publications

1. Grzywa M., Nitek W., Łasocha W., The crystal structures of lithium tetraperoxo-molybdate(VI) tetrahydrate $Li_2[Mo(O_2)_4]$ $4H_2O$ and lithium tyetraperoxotungstate(VI) tetrahydrate $Li_2[W(O_2)_4]$ ˇ$4H_2O$, J. Mol. Struct., 828, 111–115, 2007.
2. Grzywa M., Łasocha W., Structure solution from powder diffraction data – fast and fully "ab inito" study. Crystal structure of potassium and ammonium tetraperoxovanadates(V). Z. Kristallogr., 222, 95–98, 2007.
3. Grzywa M., Łasocha W., Surga W., Synthesis, characterization and crystal structure of zinc dimolybdate pentahydrate $ZnMo_2O_7.5H_2O$, J. Solid State Chem., 180, 1590–1594, 2007.
4. Włodarczyk-Gajda B., Rafalska-Łasocha A., Łasocha W., Synthesis and crystal-structure determination of fibrillar methylammonium trimolybdate, Hydrate, Powder Diffraction, 22, 241–245, 2007.
5. Gawel B., Łasocha W., Zieba M., New inorganic-organic composite ZnSe(MXDA)(1/2), J. Alloy Compd., 442, 77-79, 2007.
6. Łasocha W., Rafalska-Łasocha A., Grzywa M., Gaweł B., New achievements in X-ray techniques in the investigations of catalysts., Catal. Today, 137, 504-509, 2008.
7. Tejchman W., Zborowski K., Proniewicz L.M., Łasocha W., Selenomaltol – new ligand for coordination chemistry. Synthesis, spectroscopy and theoretical calculations, Heterocycles, 75, 1931–1942, 2008.
8. Grzywa M., Łasocha W., Rutkowska-Żbik D., Structural investigation of tetraperoxo complexes of Mo(VI) and W(VI) X-ray and theoretical studies, J. Solid State Chem., 182, 973–982, 2009.



Joanna Łojewska

Dr habil, PhD

Research profile

Chemistry of solid state; Catalysis; Cellulose chemistry; Infrared spectroscopy

My interest spreads over catalysis, conservation chemistry and molecular spectroscopy. In 2006 I became Head of the Kinetics of Heterogeneous Reactions research group.

In catalysis the effort is targeted at designing the metallic structured reactors for combustion processes. Of particular interest is the development of catalyst preparation methods and the search for nanocomposite metal oxide catalysts that could replace precious metal-containing ceramic monoliths. This research is done in cooperation with the Technical Universities of Silesia and Łódź and with the Institute of Chemical Engineering of the Polish Academy of Sciences.

In conservation chemistry the focus is on degradation processes (paper, pigments, dyes) and also on analytical methods for investigating historical objects. In this area we cooperate with a great many institutions of cultural heritage in Poland and in Europe, notable among them being the Jagiellonian Library, the National Museum and the Academy of Fine Arts in Kraków. Part of this research has been carried out within Long-Term National Project "Acidic Paper". Currently we conduct a postgraduate course of studies in Modern Analytical Techniques in Conservation Science.

More information: www.chemia.uj.edu.pl/zespol.php?id=10038

Selected publications

1. Kołodziej A., Łojewska J., Catal. Today, 105, 378–384, 2005.
2. Łojewska J., Kołodziej A., Żak J., Stoch J., Catal. Today, 105, 655–661, 2005.
3. Łojewska J., Dynarowicz-Łątka P., Kołodziej A., Thin Solid Films, 495, 299–307, 2006.
4. Łojewska J., Lubańska H., Miśkowiec P., Łojewski T., Proniewicz L.M., Appl. Phys. A, 83, 597–603, 2006.
5. Kołodziej A., Łojewska J., Chem. Eng. Proc., 46, 637–644, 2007.
6. Kołodziej A., Łojewska J., Top. Catal., 42–43, 475–480, 2007.
7. Tyczkowski J., Kapica R., Łojewska J., Thin Solid Films, 15/16, 6590–6595, 2007.
8. Łojewska J., Missori M., Lubańska A., Grimaldi P., Zięba K., Proniewicz L.M, Ccongiu Castellano A., Appl. Phys. A, 89, 883–887, 2007.
9. Łojewska J., Wasilewski J., Terelak K., Łojewski T., Kołodziej A., Catal. Commmun., 9 1833–1837, 2008.
10. Łojewska J., Kołodziej A., Łojewski T., Kapica R., Tyczkowski J., Catal. Commmun., 10 142–145, 2008.
11. Kołodziej A., Łojewska J., AIChE J, 55, 264–267, 2009.
12. Kołodziej A., Łojewska J., Chem. Eng. Process., 48, 816–822, 2009.

Marek Mac

Dr habil, PhD

Research profile

Fluorescence; Electron transfer; Fluorescence indicators

My scientific interests cover the fluorescence and triplet state quenching by inorganic and organic electron donors, leading to the radical pair. The formation of the radical pair is monitored by optical and FTIR transient spectroscopy. Simple photochemical reactions occurring after charge separation were also a subject of my investigations (dechlorination of 9,10-dichloranthracene in the presence of amines in solvents of different polarity). Additionally, the influence of the inert salts on the fate of the charge transfer pair (so called salt effects) was investigated.

My present investigations concern: (i) so called fluorescence sensors of small inorganic cations based on azaromatic compounds as fluorescing units, and (ii) trans-cis isomerisation of the dyes.

Selected publications

1. Mac M., Wirz J., Najbar J., Transient radicals formed by electron transfer between ionorganic ions and excited aromatic molecules in polar solvents, Helv. Chim. Acta, 76, 1319–1331, 1993.
2. Mac M., Kwiatkowski P., Turek A.M., Quenching of exciplex fluorescence by lithium perchlorate in acetonitrile, Chem. Phys. Lett., 250, 104–410, 1996.
3. Mac M., Milart P., Kwiatkowski P., Tokarczyk. B., Influence of lithium perchlorate on electron transfer processes occurring in bianthryl in 2-methyltetrahydrofuran, J. Lumin., 81, 199–208, 1999.
4. Mac M., Wirz J., Salt effects on the reactions of radical ion pairs formed by electron transfer quenching of triplet 2-methyl-1,4-naphthoquinone by amines. Optical flash photolysis and step-scan FTIR investigations, Photochem. Photobiol. Sci., 1, 24–29, 2002.
5. Mac M., Photodehalogenation of 9,10-dichloroanthracene induced by electron transfer fluorescence quenching with primary and tertiary amines in acetonitrile and n-hexane. Salt effect on photodechlorination process, Polish J. Chem., 77, 427–439, 2003.
6. Mac M., Tokarczyk B., Uchacz T., Danel A., Charge transfer fluorescence of benzoxazol derivatives. Investigation of solvent effect on fluorescence of these dyes, J. Photochem. Photobiol. A, 191, 32–41, 2007.
7. Mac M., Baran W., Uchacz T., Baran B., Suder M., Leśniewski S., Fluorescence properties of the derivatives of oxazolo[4,5-b]pyridyne, J. Photochem. Photobiol. A, 192, 198–196, 2007.
8. Mac M., Uchacz T., Danel A., Miranda M.A., Paris C., Pischel U., Intramolecular exciplexes based on benzoxazole: photophysics and applications as fluorescent cation sensors, Photochem. Photobiol. Sci., 7, 633–641, 2008.

Wojciech Macyk

Dr habil, PhD

Research profile

Heterogeneous photocatalysis; Photochemistry; Functional materials

Graduated from the Jagiellonian University in 1997 (supervision of Professor Zofia Stasicka), he took up PhD studies at the University of Erlangen-Nürnberg, Germany, in the group of Professor Horst Kisch, working on the photosensitization of TiO_2 by visible light. Upon completion of the PhD in 2000, he worked two more years in the same group. In 2002 he joined the Coordination and Bioinorganic Physicochemistry group at the Faculty of Chemistry, Jagiellonian University, where he completed his Habilitation in 2009. His research interests include heterogeneous photocatalysis (especially TiO_2 photosensitization and singlet oxygen generation at wide bandgap semiconductors), photocatalytic detoxification and disinfection, as well as photoelectrochemistry of nanocrystalline semiconductors. He was awarded the Albert Weller Prize and the Staedtler Prize, in addition to the fellowships from the Foundation for Polish Science and *Polityka* magazine.

Selected publications

1. Macyk W., Kisch H., Photosensitization of crystalline and amorphous titanium dioxide by Pt^{IV}-chloride surface complexes, Chem. Eur. J., 7, 1862–1867, 2001.
2. Macyk W., Burgeth G., Kisch H., Photoelectrochemical properties of platinum(IV)-chloride surface modified TiO_2, Photochem. Photobiol. Sci., 2, 322–328, 2003.
3. Szaciłowski K., Macyk W., Drzewiecka-Matuszek A., Brindell M., Stochel G., Bioinorganic photochemistry. Frontiers and mechanisms, Chem. Rev., 105, 2647–2694, 2005.
4. Macyk W., Franke A., Stochel G., Metal compounds and small molecules activation – case studies, Coord. Chem. Rev., 249, 2437–2457, 2005.
5. Szaciłowski K., Macyk W., Chemical switches and logic gates based on surface modified semiconductors, C. R. Chimie, 9, 315–324, 2006.
6. Szaciłowski K., Macyk W., Stochel G., Light-driven OR and XOR programmable chemical logic gates, J. Am. Chem. Soc., 128, 4550–4551, 2006.
7. Jańczyk A., Krakowska E., Stochel G., Macyk W., Singlet oxygen photogeneration at surface modified titanium dioxide, J. Am. Chem. Soc., 128, 15574–15575, 2006.
8. Mitoraj D., Jańczyk A., Strus M., Kisch H., Stochel G., Heczko P., Macyk W., Visible light inactivation of bacteria and fungi by modified titanium dioxide, Photochem. Photobiol. Sci., 6, 642–648, 2007.
9. Macyk W., Stochel G., Szaciłowski K., Photosensitization and the photocurrent switching effect in nanocrystalline titanium dioxide functionalized with iron(II) complexes: a comparative study, Chem. Eur. J., 13, 5676–5687, 2007.
10. Jańczyk A., Wolnicka-Głubisz A., Urbańska K., Kisch H., Stochel G., Macyk W., Photodynamic activity of platinum(IV) chloride surface-modified TiO_2 irradiated with visible light, Free Radic. Biol. Med., 44, 1120–1130, 2008.
11. Stochel G., Stasicka Z., Brindell M., Macyk M., Szaciłowski K., Bioinorganic Photochemistry, 398 pages, Wiley, 2009.

Wacław Makowski

Dr habil, PhD

Research profile

Adsorption; Heterogeneous catalysis; Thermal analysis

Head of the Research Group for Catalysis and Solid State Chemistry II

Recent scientific activity of the group is focused on the studies of porosity and surface chemistry of adsorbents and catalysts by means of thermodesorption of probe molecules. A considerable achievement in this field was an application of the quasi-equilibrated thermodesorption of n-alkanes for the characterization of micro- and mesoporous materials, including their mesopore size distribution.

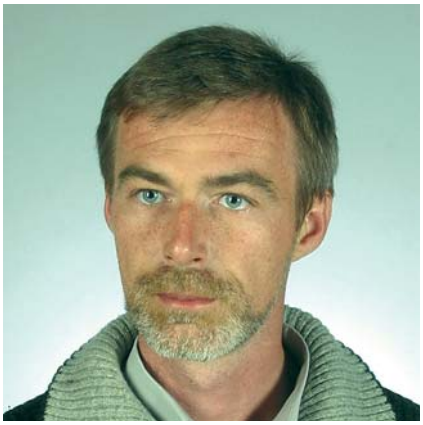
Other fields of interests cover adsorption of organic compounds on porous solids as well as catalytic applications of the materials synthesized from double-layered hydroxides.

Selected publications

1. Schulze K., Makowski W., Chyży R., Dziembaj R., Geismar G., Nickel doped hydrotalcites as catalyst precursor for the partial axidation of light paraffins, Appl. Clay Sci., 18, 59–69, 2001.
2. Makowski W., Majda D., Temperature programmed equilibrated desorption of n-hexane as a tool for characterisation of the microporous structure of zeolites, Thermochim. Acta, 412, 131–137, 2004.
3. Makowski W., Majda D., Equilibrated thermodesorption studies of adsorption of n-hexane and n-heptane on zeolites Y, ZSM-5 and ZSM-11, Appl. Surf. Sci., 252, 707–715, 2005.
4. Makowski W., Majda D., Temperature programmed desorption of n-hexane and n-heptane from MFI and FAU zeolites, J. Porous Mat., 14, 27–35, 2007.
5. Makowski W., Quasi equilibrated temperature programmed desorption and adsorption – a new method for determination of the isosteric adsorption heat, Thermochim. Acta, 454, 26–32, 2007.
6. Makowski W., Kuśtrowski P., Probing pore structure of microporous and mesoporous molecular sieves by quasi-equilibrated temperature programmed desorption and adsorption of n-nonane, Micropor. Mesopor. Mat., 102, 283–289, 2007.
7. Makowski W., Ogorzałek Ł., Determination of the adsorption heat of n-hexane and n-heptane on zeolites beta, L, 5A, 13X, Y and ZSM-5 by means of quasi equilibrated temperature programmed desorption and adsorption (QE-TPDA) , Thermochim. Acta, 465, 30–39, 2007.
8. Makowski W., Gil B., Majda D., Characterization of acidity and porosity of zeolite catalysts by the equilibrated thermodesorption of n-hexane and n-nonane, Catal. Lett., 120, 154–160, 2008.
9. Makowski W., Chmielarz L., Kuśtrowski P., Determination of the pore size distribution of mesoporous silicas by means of quasi-equilibrated thermodesorption of n-nonane, Micropor. Mesopor. Mat., 120, 257–262, 2009.

Artur Michalak

Professor of Chemistry, Dr habil, PhD



Research profile

Theoretical chemistry; Polymerization of olefins; Chemical bonding

The *Molecular Modelling of Catalytic Processes* group (Professor A. Michalak, M. Mitoraj, PhD, M. Srebro, A. Rogowska, Ł. Piękoś) specializes in theoretical studies covering various aspects of catalysis. Recent scientific interests has been focused on: (i) DFT modelling of the polymerization processes catalyzed by TM complexes, within which theoretical analysis of the factors controlling the activity of TM-complexes as catalysts for polymerization of ethylene and α-olefins and for their copolymerization with polar-group containing monomers, is performed; (ii) Relationship between the catalyst structure and activity; (iii) Influence of the catalyst structure on the polyolefin branching and mictrostructure.

Current research interest also involves description of chemical bonding. In particular, new sets of orbitals have been proposed: *The Natural Orbitals for Chemical Valence* (NOCV), and *Localized Orbitals from Bond-Order Operator* (LOBO).

Professor Artur Michalak is an author of 57 scientific publications, including 6 monographic chapters; total number of citations >900; Hirsch-index is 19.

Selected publications

1. Michalak A., Ziegler T., DFT Studies on the copolymerization of α-olefins with polar monomers: Ethylene-methyl acrylate copolymerization catalyzed by a Pd-based diimine catalyst, J. Am. Chem. Soc., 123, 12266–12278, 2001.
2. Michalak A., Ziegler T., Stochastic simulations of polymer growth and isomerization in the polymerization of propylene catalyzed by Pd-based diimine catalysts, J. Am. Chem. Soc., 124, 7519–7528, 2002.
3. Haras A., Michalak A., Rieger B., Ziegler T., Theoretical analysis of factors controlling the non-alternating CO/C_2H_4 copolymerization, J. Am. Chem. Soc., 127, 8765–8774, 2005.
4. Szabo M.J., Galea N.M., Michalak A., Sheng-Yong Yang, Groux L.F., Piers W. E., Ziegler T., Copolymerization of ethylene with polar monomers: Chain propagation and side reactions. A DFT theoretical study using zwitterionic Ni(II) and Pd(II) catalysts, J. Am. Chem. Soc., 127, 14692–14703, 2005.
5. Michalak A., Ziegler T., Pd-catalyzed polymerization of propene – DFT model studies, Organometallics, 18, 3998–4004, 1999.
6. Michalak A., Ziegler T., DFT studies on substituent effects in Pd-catalyzed olefin polymerization, Organometallics, 19, 1850–1858, 2000.
7. Mitoraj M., Michalak A., Natural orbitals for chemical valence as descriptors of chemical bonding in transition metal complexes, J. Mol. Model., 13, 347–355, 2007.
8. Mitoraj M., Michalak A., Donor-acceptor properties of ligands from the natural orbitals for chemical valence, Organometallics, 26, 6576–6580, 2007.
9. Michalak A., Mitoraj M., Ziegler T., Bond-orbitals from chemical valence theory, J. Phys. Chem. A, 112, 1933–1939, 2008.

Anna Migdał-Mikuli

Professor of Chemistry, Dr habil, PhD

Research profile

I. Chemical education; II. Chemical physics; Molecular reorientation and vibration; Calorimetry; Phase transitions; Molecular, plastic, liquid, co-ordination and ionic crystals

I. As Head of Chemical Education Department, she realizes a research programme that revolves mainly around the blended learning system issue. The system incorporates many different learning styles that can be accomplished through mixing classical learning and distance learning elements. Classical teaching has been enriched by using the interactive teaching environment (interactive board, personal response system). The department carries out the assessment of the effectiveness of teaching that uses both the classical and the blended method. *Co-workers*: Michał Poźniczek, PhD, Zofia Kluz, PhD, Paweł Broś, MSc, Paweł Bernard, MSc.

II. As a member of the *Phase Transitions* research group, she is mainly interested in properties of molecular, plastic, liquid and coordination ionic crystals. Special attention is focused on liquid and plastic crystal phases. Measurements in a temperature range of 20–400 K are performed by means of complementary methods, such as inelastic and *quasi*-elastic neutron scattering, infrared and Raman spectroscopies, nuclear magnetic resonance, X-ray and neutron diffraction, thermogravimetry and differential scanning calorimetry. *Co-workers*: Elżbieta Szostak, PhD, Joanna Hetmańczyk, PhD, Łukasz Skoczylas, MSc, Diana Dołęga, MSc.

More information: www.chemia.uj.edu.pl/migdalmi

Selected publications

1. Migdał-Mikuli A., Broś, P., Bernard P., Purpose and form realization of the blended learning system during chemistry academic courses, Problems of Education in the 21st century, Information and Communication Technology in Education: Opportunities and Challenges, 5, 98–104, 2008.
2. Migdał-Mikuli A., Bernard P., Preparation of support materials for specialist courses for chemistry students, Ann. Polish Chem. Soc., 362–365, 2007.
3. Migdał-Mikuli A., Hetmańczyk J., Thermal behavior of $[Ca(H_2O)_4](ClO_4)_2$ and $[Ca(NH_3)_6](ClO_4)_2$, J. Therm. Anal. Calorim., 91, 529–534, 2008.
4. Migdał-Mikuli A., Szostak E., Drużbicki K., Dołęga D., Polymorphism and thermal decomposition of $[Ni(DMSO)_4]I_2$, J. Therm. Anal. Calorim., 93, 853–856, 2008.
5. Migdał-Mikuli A., Hołderna-Natkaniec K., Mikuli E., Hetmańczyk Ł., Natkaniec I., Phase transitions and NH_3 motions in $[Zn(NH_3)_4](ClO_4)_2$ studied by incoherent neutron scattering and ^1H NMR methods, Chem. Phys., 335, 187–193, 2007.
6. Migdał-Mikuli A., Szostak E., Polymorphism of $[Ni(DMSO)_{6]}(ClO_4)_2$ studied by differential scanning calorimetry, Z. Naturforsch., 62a, 67–74, 2007.
7. Migdał-Mikuli A., Hetmańczyk J., Hetmańczyk Ł., Thermal behaviour of $[Ca(H_2O)_4](NO_3)_2$, J. Therm. Anal. Calorim., 89, 499–503, 2007.

Edward Mikuli

Professor of Chemistry, Dr habil, PhD

Research profile

Chemical physics; Molecular spectroscopy; Neutron scattering; Calorimetry; Phase transitions; Vibrational and reorientational dynamics; Molecular, plastic, liquid, coordination crystals; Orientational and structural glasses

Scientific interests of the *Phase Transitions* research group (Professor Edward Mikuli (Head), Łukasz Hetmańczyk, PhD, Elżbieta Szostak, PhD, Joanna Hetmańczyk, PhD, Marta Liszka-Skoczylas, MSc, Łukasz Skoczylas, MSc, Diana Dołęga, MSc, Kacper Drużbicki, MSc) focus on investigating phase transitions in coordination, molecular, plastic and liquid crystals. The connections between phase transitions and the change of molecular dynamics and/or crystal structure are determined, and the thermodynamic parameters of phase transitions and reorientational correlation times are calculated. Measurements in wide range of temperature (20–400 K) are performed by means of complementary methods, such as inelastic and *quasi*-elastic neutron scattering, infrared and Raman spectroscopies, nuclear magnetic resonance, X-ray and neutron diffraction, thermogravimetry and differential scanning calorimetry. Additionally, for the full interpretation of the molecular spectra, quantum chemical calculations are carried out.

More information: www.chemia.uj.edu.pl/~mikuli

Selected publications

1. Migdał-Mikuli A., Mikuli E., Hetmańczyk J., Hetmańczyk Ł., Hołderna-Natkaniec K., Natkaniec I., Phase transitions and H_2O motions in $[Ca(H_2O)_4](NO_3)_2$ studied by infrared spectroscopy, inelastic/quasielastic incoherent neutron scattering and proton magnetic resonance, Part II, J. Alloy. Compd., 469, 73–81, 2009.
2. Hetmańczyk J., Hetmańczyk Ł., Migdał-Mikuli A., Mikuli E., Nitek W., Phase transitions in $[Ca(H_2O)_4](ClO_4)_2$ studied by differential scanning calorimetry, X-ray single crystal diffraction and neutron powder diffraction, J. Mol. Struct., 891, 233–241, 2008.
3. Mikuli E., Hetmańczyk Ł., Medycki W., Kowalska A., Phase transitions and molecular motions in $[Zn(NH_3)_4](BF_4)_2$ studied by nuclear magnetic resonance, infrared and Raman spectroscopy, J. Phys. Chem. Solids, 68, 96–103., 2007.
4. Migdał-Mikuli A., Hołderna-Natkaniec K., Mikuli E., Hetmańczyk Ł., Natkaniec I., Phase transitions and NH_3 motions in $[Zn(NH_3)_4](ClO_4)_2$ studied by incoherent neutron scattering and ^1H NMR methods, Chem. Phys., 335, 187–193, 2007.
5. Mikuli E., Szostak E., Grad B., Phase transitions in $[Mg(H_2O)_6](BF_4)_2$ studied by differential scanning calorimetry, Phase Transit., 80, 539–546, 2007.
6. Migdał-Mikuli A., Mikuli E., Hetmańczyk Ł., Natkaniec I., Ściesiński J., Ściesińska E., Wróbel S., Phase transition, molecular motions and structural changes and low-frequency vibrations in $[Cu(NH_3)_5](ClO_4)_2$, Chem. Phys., 317, 188–197, 2005.
7. Mikuli E., Grad B., Medycki W., Hołderna-Natkaniec K., Phase transitions and molecular motions in $[Cd(H_2O)_6](BF_4)_2$ studied by DSC, ^1H & ^{19}F NMR and FT-MIR, J. Solid State Chem., 177, 3795–3804, 2004.

Jacek Młynarski

Dr habil, PhD

Research profile

Asymmetric synthesis; Metal complexes; Organocatalysis

PhD, Institute of Organic Chemistry, Polish Academy of Sciences, Warsaw, 2000;
Post-doc, MPI, Mülheim a.d. Ruhr, Germany, 2001–2002 (Professor Alois Fürstner), Alexander von Humboldt Fellowship, 2001;
Habilitation, Institute of Organic Chemistry, Polish Academy of Sciences, Warsaw, 2006, Professor at the Faculty of Chemistry, Jagiellonian University, 2009.

Research of Młynarski group in broad terms focuses on organic synthesis and the discovery of new reaction methodology, in particular on stereoselective and catalytic asymmetric reactions. Inventing new strategies for the development of perfect chemical reactions, as part of the green chemistry concept, is the ultimate goal of our research. Currently our interest involves enantioselective synthetic methodology relying on both metal-based chiral catalysts and purely organic molecules, and includes:

1. Development of water-compatible chiral Lewis acids.
2. Designing of new catalysts for direct asymmetric aldol and aldol-type reactions in water. Biomimetic concept.
3. Synthesis of novel type chiral ligands for aqua-asymmetric carbon-carbon bond formations (designing of water-compatible chiral Zn and Fe complexes).
4. Towards enzyme mimics: direct aldol reaction in water promoted by chiral Zn(II) complexes and by small organic molecules.

More information: www.jacekmlynarski.pl

Selected publications

1. Paradowska J., Stodulski M., Młynarski J., Asymmetric catalysis in water mediated by amino acids-based catalysts, Angew. Chem. Int. Ed., in press, 2009.
2. Młynarski J., Paradowska J., Catalytic asymmetric aldol reactions in aqueous media, Chem. Soc. Rev., 37, 1502–1511, 2008.
3. Paradowska J., Stodulski M., Młynarski J., Direct catalytic asymmetric aldol reactions assisted by zinc complex in the presence of water, Adv. Synth. Catal., 239, 1041–1046, 2007.
4. Jankowska J., Paradowska J., Rakiel B., Młynarski J., Iron(II) and zinc(II) complexes with designed pybox ligands for the asymmetric aqueous Mukaiyama-aldol reactions, J. Org. Chem., 72, 2228–2231, 2007.
5. Młynarski J., Rakiel B., Stodulski M., Suszczyńska A., Frelek J., The chiral ytterbium complexes-catalyzed direct asymmetric aldol-Tishchenko reaction. Synthesis of anti-1,3-diols, Chem. Eur. J., 12, 8158–8167, 2006.
6. Jankowska J., Młynarski J., Zn(pybox)-Complex catalyzed asymmetric aqueous Mukaiyama-aldol reactions, J. Org. Chem., 71, 1317–1321, 2006.

Janusz Mrozek

Dr habil, PhD

Research profile

Theory of valency; Electronic structure theory; Relations between electronic structure and geometry of closed and open molecular systems; Hybrid optimization algorithms

Current research interests concentrate on:

(1) Applications of information theory to the theory of chemical valency. This includes both computing the ionic and covalent bond order indices based on the analysis of molecular communication channels and exploring molecular bonding regions (in physical space) with use of the kinetic energy (contragradience) criterion, related to the non-additive Fisher information.

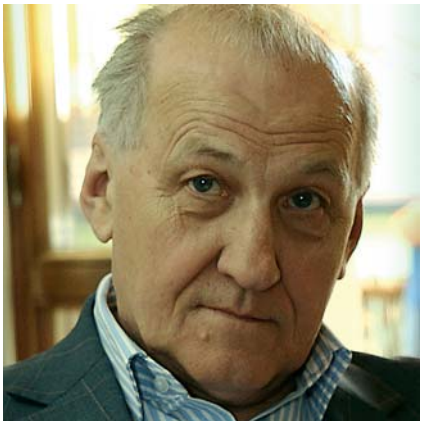
(2) Exploration within the Born–Oppenheimer approximation of the compliance constants reflecting the coupling between molecular electronic and geometric degrees-of-freedom for both the externally closed and open molecular systems.

(3) Applications of hybrid optimization algorithms (gradient, genetic algorithms and neural network) to the conformational analysis of molecular systems.

Research on chemical valency is a continuation of previous work on valence indices from the two-particle density matrix.

Selected publications

1. Nalewajski R.F., Błażewicz D., Mrozek J., Math. Chem., 44, 325–364, 2008.
2. Nalewajski R.F., Mrozek J., Int. J. Quantum Chem., 51, 187–200, 1994.
3. Nalewajski R.F., Formosinho S.J., Varandas A.J.C., Mrozek J., Int. J. Quantum Chem., 52, 1153–1176, 1994.
4. Nalewajski R.F., Mrozek J., Int. J. Quantum Chem., 57, 377–389, 1996.
5. Nalewajski R.F., Mrozek J., Michalak A., Int. J. Quantum Chem., 61, 589–601, 1997.



Jan Najbar

Professor of Chemistry, Dr habil, PhD

Research profile

Radiationless transitions; Heavy-atom effects; Photoinduced electron transfer; Supersonic-jet; Laser induced fluorescence; Geometry electronically excited organic molecules

The Photochemistry and Luminescence group members are Andrzej M Turek, Dr habil, PhD, and Przemysław Kolek, PhD. Research carried out by our group is in the field of physical chemistry related to photophysics and photochemistry of organic molecules, and to laser spectroscopy. In particular, we perform studies of intramolecular and intermolecular interactions influencing the rates of radiative and radiationless processes. The emphasis is on the early events that follow light absorption and the spin-orbit interactions in molecules and in weak complexes. Our research topics include: (i) the ultrafast electron transfer processes and salvation dynamics, (ii) spectroscopy of jet-cooled organic molecules, (iii) laser induced fluorescence, (iv) deuteration effects, (v) theory of ultrafast photochemical reactions in solutions, (vi) charge separation phenomena in triad systems, (vi) effects of the electric field on electron transfer reactions, (vii) roles of the spin dynamics in multistep electron transfer processes.

Selected publications

1. Najbar J., Birks J.B., Hamilton T.D.S., The influence of iodide ions on radiative $T_1 \rightarrow S_0$ transition in aromatic hydrocarbons, Chem. Phys., 23, 281–294, 1977.
2. Jarzęba W., Najbar J., Ciosłowski J., Internal heavy-atom effects for chloro- and bromo-quinolines, J. Mol. Struct., 141, 469–474, 1986.
3. Najbar J., Dorfman R.C., Fayer M.D., Solvent relaxation effects in transient kinetics of photo-induced electron transfer reactions, J. Chem. Phys., 94, 1081–1092, 1991.
4. Najbar J., Jarzęba W., Rate coefficients for the electron transfer in symmetrical systems, Chem. Phys. Letters, 196, 504–510, 1992.
5. Najbar J., Tachiya M., Potential energy surfaces for supramolecular triad system A-D-A in polar solvent, J. Phys. Chem., 98, 199–205, 1994.
6. Mac M., Najbar J., Wirz J., Fluorescence and intersystem crossing from the twisted intramolecular charge transfer (TICT) state of bianthryl in the presence of inorganic ions in polar solvents, J. Photochem. Photobiol. A, 88, 93–104, 1995.
7. Najbar J., Tachiya M., Solvent effects on the electron transfer reactions in supramolecular systems, J. Photochem. Photobiol. A, 95, 51–59, 1996.
8. Kolek P., Pirowska K., Chacaga Ł, Najbar J., LIF excitation spectra of jet-cooled 3,5-dicyanoaniline, Phys. Chem. Chem. Phys., 5, 4096–4107, 2003.
9. Leśniewski S., Kolek P., Pirowska K., Sobolewski A., Najbar J., Franck-Condon analysis of laser-induced fluorescencje excitation spectrum of anthranilic acid: Evaluation of geometry change upon $S_0 \rightarrow S_1$ excitation, J. Chem. Phys., 130, 054307, 2009.

Mieczysława Najbar

Professor of Chemistry, Dr habil, PhD

Research profile

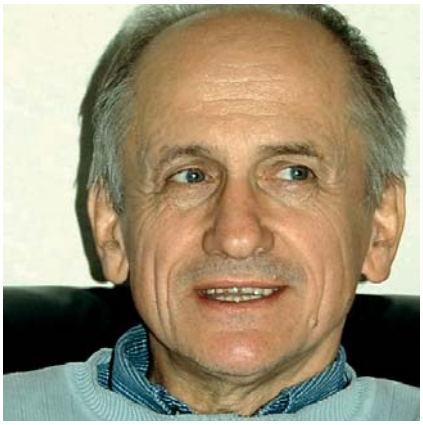
Solid state chemistry and heterogeneous catalysis on oxides and metals

Associate researcher at Lehigh University, Bethlehem, USA, 1986–1987 and National Institute of Materials and Chemical Research, Tsukuba, Japan, 1995; Main organizer of Polish Seminars on Catalytic DENOX (1993–1996) and of International Symposia on Air Pollution Abatement; Guest Editor of Polish Journal of Environmental Studies and of Catalysis Today

Research topics: Cation and phase segregation induced by redox processes in oxide systems and in alloys (XPS, Raman spectroscopy, X-ray microprobe analysis HRTEM, powder XRD and electron diffraction); Methane oxy-reforming and light hydrocarbons' total oxidation on Pd, Ru, Rh and Rh-Al alloys; NH_3-SCR of NO on vanadia based catalysts; NO direct decomposition to dinitrogen and dioxygen on vanadia based catalysts and on low loaded Rh/δ Al_2O_3 catalysts; Oxidation of CO and diesel soot particulates on MnO_2-based catalysts.

Selected publications

1. Bielański A., Najbar M., V_2O_5-MO_3 catalysts for benzene oxidation, Appl. Catal. A-Gen., 157, 223–261, 1997.
2. Najbar M, Camra J., Białas A., Wesełucha-Birczyńska A., Borzęcka-Prokop B., Delevoye L., Klinowski J., Structural studies of V_2O_5-WO_3 and WO_3-V_2O_5 solid solutions, Phys. Chem. Chem. Phys., 1, 4645–4648, 1999.
3. Camra J., Bielańska E., Bernasik A., Kowalski K., Zimowska M., Białas A., Najbar M., Role of Al segregation and high affinity to oxygen in formation of adhesive alumina layers on FeCr alloy support, Catal. Today, 105, 629–633, 2005.
4. Zimowska M., Wagner J. B., Dziedzic J., Camra J., Borzęcka-Prokop B., Najbar M., Some aspects of metal-support strong interactions in Rh/Al_2O_3 catalyst under oxidising and reducing conditions, Chem. Phys. Lett., 417,137–142, 2006.
5. Pietraszek A., Da Costa P., Marques R., Kornelak P., Hansen T.W., Camra J., Najbar M., The effect of the Rh–Al, Pt–Al and Pt–Rh–Al surface alloys on NO conversion to N_2 on alumina supported Rh, Pt and Pt–Rh catalysts, Catal. Today, 119, 187–193, 2007.
6. Banas J., Tomašic V., Weselucha-Birczynska A., Najbar M., Structural sensitivity of NO decomposition over a V-O-W/Ti(Sn)O_2 catalyst, Catal. Today, 119, 199–203, 2007.
7. Białas A., Osłuch W., Łasocha W., Najbar M., The influence of Cr-Al foil texture on morphology of adhesive Al_2O_3 layers in monolithic environmental catalysts, Catal. Today, 137, 489–492, 2008.
8. Kornelak P., Su D., Thomas C., Dobrzyńska-Lityńska L., Bielańska E., Camra J., Wesełucha-Birczyńska A., Najbar M., Surface species structure and activity in NO decomposition of anatase supported V-O-Mo catalyst, Catal. Today, 137, 273–277, 2008.



Roman F. Nalewajski

Professor of Chemistry, Dr habil, PhD

Research profile

Theoretical chemistry; Quantum chemistry; Chemical physics; Theory of chemical reactivity and catalysis; Information theory of molecular systems and their fragments

Current scientific interests: (i) Density Functional Theory of molecular and reactive systems (ii) Theory of chemical valence and bond multiplicities; (iii) Applications of Information Theory in extracting chemical interpretation of molecular electronic structures: entropic principles for subsystems, information origins of the chemical bond, thermodynamic-like description of electrons in molecules.

Selected publications

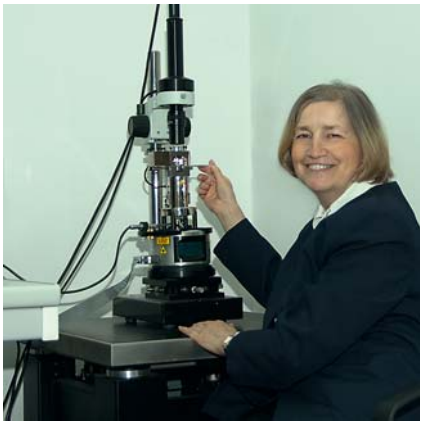
1. Nalewajski R.F., Parr R.G., Information theory, atoms-in-molecules and molecular similarity, Proc. Natl. Acad. Sci. USA, 97, 8879–8882, 2000.
2. Nalewajski R.F., Entropic measures of bond multiplicity from the information theory, J. Phys. Chem. A, 104, 11940–11951, 2000.
3. Nalewajski R.F., Information theoretic approach to fluctuations and electron flows between molecular fragments, J. Phys. Chem. A, 107, 3792–3802, 2003.
4. Nalewajski R.F., Electronic structure and chemical reactivity: Density functional and information theoretic perspectives, Adv. Quant. Chem., 43, 119–184, 2003.
5. Nalewajski R.F., Köster A.M., Escalante S., Electron localization function as information measure, J. Phys. Chem. A, 109, 10038–10043, 2005.
6. Nalewajski R.F., Probing the interplay between electronic and geometric degrees-of-freedom in molecules and reactive systems, Adv. Quant. Chem., 51, 235–305, 2006.
7. Nalewajski R.F., Broniatowska E., Atoms-in-molecules from the stockholder partition of the molecular *two*-electron distribution, Theor. Chem. Acc., 117, 7–27, 2007.
8. Nalewajski R.F., Chemical bonds through probability scattering: Information channels for intermediate-orbital stages, J. Math. Chem., 43, 780–830, 2008.
9. Nalewajski R.F., Internal and external eigenvalue problems of hermitian operators and their use in electronic structure theory, J. Math. Chem., 44, 802–815, 2008.
10. Nalewajski R.F., Use of Fisher information in quantum chemistry, Int. J. Quantum Chem. 108, 2230–2252, 2008.
11. Nalewajski R.F., Multiple, localized and delocalized/conjugated bonds in the orbital communication theory of molecular systems, Adv. Quant. Chem., 56, 217–250, 2009.

Books

1. Nalewajski R.F., Korchowiec J., Charge Sensitivity Approach to Electronic Structure and Chemical Reactivity, World Scientific, Singapore, 1997.
2. Nalewajski R.F., Foundations and Methods of Quantum Chemistry: Lectures, PWN, Warszawa, 2001 (In Polish).
3. Nalewajski R.F. (Ed.), Density Functional Theory I–IV, Topics in Current Chemistry, vols 180–183, Springer-Verlag, Heidelberg, 1996.
4. Nalewajski, R.F., Information Theory of Molecular Systems, Elsevier, Amsterdam, 2006.

Maria Nowakowska

Professor of Chemistry, Dr habil, PhD



Research profile

Physical chemistry; Materials science; Photophysics and photochemistry; Nanochemistry and nanotechnology

Professor M. Nowakowska is a specialist in physical chemistry. Her field of research involves nanochemistry, new materials, supramolecular chemistry, photophysics and photochemistry of polymers, environmental issues and advanced materials for biomedical applications. Her research group of Nanotechnology of Polymers and Biomaterials includes several world class young researchers, and is constantly attracting PhD, MSc and undergraduate students. The group is involved in wide scientific collaboration with Polish and foreign partners from academia, industry, teaching hospitals and medical centers. The laboratories of the group are very well equipped with modern instruments, and the research is published in prestigious international scientific journals or patented. More information on the research profile, group activity, current programmes, openings and funding is available at: www.chemia.uj.edu.pl/zespol.php?id=10019.

Selected publications

1. Kamiński K., Zazakowny K., Szczubiałka K., Nowakowska M., Biomacromolecules, 9, 3127–3132, 2008.
2. Nawalany K., Kozik B., Kępczyński M., Zapotoczny S., Humorek M., Nowakowska M., Jachimska B., J. Phys. Chem. B, 112, 12231–12239, 2008.
3. Zapotoczny S., Golonka M., Nowakowska M., Langmuir, 24, 5868–5876, 2008.
4. Nowakowska M., Moczek L., Szczubiałka K., Biomacromolecules, 9, 1631–1636, 2008.
5. Zapotoczny S., Rymarczyk-Machał M., Stradomska A., Petelenz P., Nowakowska M., J. Phys. Chem. B, 111, 10088–10094, 2007.
6. Kępczyński M., Lewandowska J., Romek M., Zapotoczny S., Ganachaud F., Nowakowska M., Langmuir, 23, 7314–7320, 2007.
7. Moczek Ł., Nowakowska M., Biomacromolecules, 8, 433–438, 2007.
8. Rymarczyk-Machał M., Zapotoczny S., Nowakowska M., J. Polym. Sci. A, 44, 2675–2683, 2006.
9. Zapotoczny S., Golonka M., Nowakowska M., Macromol. Rapid Commun., 26, 1049–1054, 2005.
10. Kępczyński M., Karewicz A., Górnicki A., Nowakowska M., J. Phys. Chem. B., 109, 1289–1294, 2005.
11. Nowakowska M., Sterzel M., Zapotoczny S., Kot E., Appl. Catal. B, 57, 1–8, 2005.
12. Nowakowska M., Zapotoczny S., Sterzel M., Kot E., Biomacromolecules, 5, 1009–1014, 2004.
13. Nowakowska M., Karewicz A., Kłos M., Zapotoczny S., Macromolecules, 36, 4134–4139, 2003.
14. Nowakowska M., Zapotoczny S., Karewicz A., Macromolecules, 33, 7345–7348, 2000.
15. Guillet J.E., Nowakowska M., US Patent 7,345,166 B2, USA, 18 March 2008.

Barbara J. Oleksyn

Professor of Chemistry, Dr habil, PhD

Research profile

Crystallography; Crystal chemistry; Structure-biological activity relationships; Antimalarials; Potential anti-HIV-1, anticancer, antifungal and other drugs

Consultant of the Teaching Commission of the International Union of Crystallography, 1981–1984; Member, 1984–1987, and Consultant, 1988–1991, of the Commission of Small Molecules of the International Union of Crystallography; Chairman of the Kraków Division of the Polish Chemical Society, 1993–1997, Vice-Dean for Students Affairs, Faculty of Chemistry, 1996–1999; Treasurer of the Polish Crystallographic Society, 2006–2009; Supervisor of ten PhD students.

In the Crystal Chemistry of Drugs research group (Agnieszka Skórska-Stania, PhD, Justyna Kalinowska-Tłuścik, PhD, and Jan Śliwiński, MSc) we concentrate on studies of the relationship between molecular structure and activity of drugs and potential drugs, especially antimalarials. The information provided by crystal structure investigations on molecular geometry, absolute configuration, conformation and intermolecular interactions, enables us to find the features essential for the biological properties of the studied compounds. We also systematically examine the mutual influence of crystalline environment and molecular geometry of certain compounds with interesting properties, e.g. of dibenzotetraaza[14]annulenes and their metal complexes. Recently we have undertaken structural studies of ceramic biomaterials and drug delivery systems. Most of our work is carried out in co-operation with other research groups in Poland and abroad.

Selected publications

1. Kalinowska-Tłuścik, J., Jarzembek K., Śliwiński J., Oleksyn B.J., Kozik V., Polański J., Bitter sweeteners: Tetrazole derivatives of arylsulfonylalcanoids – Synthesis, structure and comparative study, Acta Crystallogr. B, 64, 760–770, 2008.
2. Zeslawska E., Stűrzebecher J., Oleksyn B.J., Geometry of gPPE binding to picrate and to the urokinase type plasminogen activator, Bioorg. Med. Chem. Lett., 17, 6212–6215, 2007.
3. Tesarowicz I., Oleksyn B.J., Nitek W., Crystal and molecular structures of trichloro-cobalt (II) complexes of epiquinine, epiquinidine, and epidihydrocinchonine, Chirality, 19, 152–161, 2007.
4. Musioł R., Jampilek J., Buchta V., Silva L., Niedbala H., Podeszwa B., Palka A., Majerz-Maniecka K., Oleksyn B., Polanski J., Antifungal properties of new series of quinoline derivatives, Bioorg. Med. Chem., 14, 3592–3598, 2006.
5. Skórska A., Stadnicka K., Oleksyn B.J., Cobalt complexes with cinchonidine and quinidine: Effect of C8/C9 stereochemistry and 6-substitution on intermolecular interactions, Chirality, 17, 73–78, 2005.
6. Śliwiński J., Eilmes J., Oleksyn B., Stadnicka K., Conformational polymorphism and aromaticity in crystalline dibenzotetraaza[14]annulene derivatives, J. Mol. Struct. 694, 1–19, 2004.

Andrzej Parczewski

Professor of Chemistry, Dr habil, PhD

Research profile

Analytical chemistry; Forensic research; Chemometrics

MSc 1965; PhD 1972; Habilitation 1976; Professor 1987; Full Professor 1992; Member of the Board of the Committee of Analytical Chemistry of the Polish Academy of Sciences; Head of the Commission of Chemometrics and Chemical Metrology of the Polish Academy of Sciences; Expert of the National Accreditation Commission.

Research areas: (i) Development and optimization of analytical methods and their application in environmental analysis (e.g. trace elements in the environment of the Tatra Mountains) and in forensic problems (e.g. drug profiling, investigation of fingerprints, toners for printing and copying machines, inks, glass particles); (ii) Development and application of chemometric methods for a design of experiments and optimization of analytical procedures, analysis of multidimensional data structure and for examination of interference effects in chemical analysis.

Cooperation: Institute of Forensic Research, Kraków; Institute of General and Ecological Chemistry of Technical University of Łódź; Institut für Anorganische und Analytische Chemie Friedrich-Schiller-Universität Jena, Germany.

Selected publications

1. Parczewski A., Kraft J., Einax J.W., Examination and presentation of element distribution in soil, J. Soils & Sediments, 4, 170–176, 2004.
2. Kraj A., Świst M., Strugała A., Parczewski A., Silberring J., Fingerprinting of 3,4-methylenedioxymethamphetamine markers by desorption/ionization on porous silicon, Eur. J. Mass Spectrom., 12, 253–259, 2006.
3. Szynkowska M.I., Czerski K., Grams J., Paryjczak T., Parczewski A., Preliminary studies using scanning mass spectrometry (TOF-SIMS) in the visualisation and analysis of fingerprints, Imaging Sci. J., 55, 180–187, 2007.
4. Kochana J., Tomaszewski W., Moszczyński T., Zakrzewska A., Parczewski A., Application of carbon adsorbents for extraction of MDMA impurities in TLC drug profiling, J. Liq. Chromatogr. R. T., 31, 819–827, 2008.
5. Pawluk-Kołc M., Zięba-Palus J., Parczewski A., The effect of re-annealing on the distribution of refractive index in a windscreen and windowpane classification of glass samples, Forensic Sci. Int., 174, 222–228, 2008.
6. Kochana J., Gala A., Parczewski A., Adamski J., Titania sol-gel-derived tyrosinase-based amperometric biosensor for determination of phenolic compounds in water samples. Examination of interference effects, Anal. Bioanal. Chem., 391, 1275–1281, 2008.
7. Szynkowska M.I., Czerski K., Rogowski J., Paryjczak T., Parczewski A., ToF-SIMS application in the visualization and analysis of fingerprints after contact with amphetamine drugs, Forensic Sci. Int., 184, e24–e26, 2009.

Marek Teofil Pawlikowski

Professor of Chemistry, Dr habil, PhD

Research profile

Vibronic coupling, Jahn-Teller Franck-Condon effects; Resonance Raman scattering; Circular dichroism

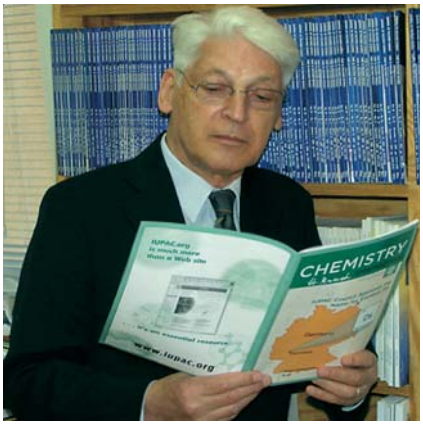
The main field of interest: (i) The theoretical studies concerning the Franck-Condon, Jahn-Teller and vibronic coupling effects in the excited states of molecules and molecular dimmers; (ii) The developments and applications of the vibronic coupling theory in the natural circular dichroism (CD), the magnetic circular dichroism and the resonance Raman (RR) spectroscopies; (iii) The interpretations and simulations of CD, MCD and RR spectra in terms of modern CASSCF and DFT methods; (iv) Pioneering works on the vibronic theory of MVCD phenomenon.

Scientific career and education: MSc, 1973, Jagiellonian University, Department of Theoretical Chemistry; PhD, 1978; Habilitation, 1989; Associate Professor, 1997; Full Professor, 2006; Postdoctoral fellowship at University of Illinois at Chicago, USA, 1983–84; Visiting Professor at National Research Council of Canada, Ottawa, 1982, 1984,1988,1993, 1995,1998 and Odense University, Department of Physics, Odense, Denmark, 1988,1989,1991,1992.

Selected publications

1. Pilch M., Pawlikowski M.T., Circular dichroism (CD) study of peridinin-chlorophyll a protein (PCP) complexes from marine dinoflagellate algae, J. Chem. Soc., Faraday T., 94, 227–232, 1998.
2. Andruniow T., Pawlikowski M., Zgierski M.Z., Density functional study of absorption and resonance Raman spectra of pyromellitic diahydride (PMDA) anion, J. Phys. Chem. A, 104, 845–851,2000.
3. Makowski M., Pilch M., Pawlikowski M.T., Circular dichroism and absorption studies of (-)-2,2'-dimethyl-4,5-(1-naphthyl)-1,3-dioxolane in terms of vibronic coupling theory, Chirality, 14, 274–284, 2002.
4. Makowski M., Pawlikowski M.T., Absorption, resonance and the preresonance Raman study of the 1,3-dicyanomethylene croconate dianion using complete active space self-consistent field and the density functional theory methods, J. Chem. Phys., 119, 12795–12804, 2003.
5. Sterzel M., Andrzejak M., Pawlikowski M.T., Gawronski J., Absorption and magnetic circular dichroism (MCD) studies of the 1,4,5,8-naphthalenetetracarboxy diimides in terms of CASSCF and DFT methods, Chem. Phys., 300, 93–105, 2004.
6. Makowski M., Pawlikowski M.T., Franck-Condon and Jahn-Teller coupling in the E_1' state of $(CO)_5^{2-}$ molecule. Resonance and preresonance Raman study in terms of time dependent density functional theory: New insight into an old story, Int. J. Quantum Chem., 104, 589–601, 2005.
7. Zazakowny P., Makowski M., Pawlikowski M.T., The Jahn-Teller effect in the E ($\pi\pi^*$) state of the $(CO)_4^{2-}$ molecule. The resonance and preresonance Raman studies in terms of time dependent density functional theory and CASSCF approach, Chem. Phys. Lett., 418, 555–560, 2006.

Stanisław Penczek



Professor of Chemistry, Honorary Professor of the Jagiellonian University, Dr habil, PhD

Research profile

Polymer chemistry; Reaction kinetics; Biomacromolecules and biopolymers

Stanisław Penczek is a polymer chemist directing research at the Centre for Molecular and Macromolecular Studies of the Polish Academy of Sciences in Łódź and teaching at the Faculty of Chemistry of the Jagiellonian University in Kraków. He got his education in Poland (Technical University, Łódź), France (CNRS, Paris), the former USSR (USSR Academy of Sciences) and in the USA (Syracuse University, NY). In addition to his research in kinetics and mechanisms of polymerization and in the synthesis of macromolecules of sophisticated architectures, he is also known for establishing several polymerization mechanisms, quoted in the major polymer textbooks. He authored and co-authored over 300 scientific papers, a number of monographs, e.g. Models of Biopolymers, CRS, 1990, Cationic Ring-Opening Polymerization, Springer, 1995, and several chapters in monographs and encyclopedias. His papers were cited over 3000 times, half of which during the last five years.

Professor Penczek is co-Editor in Chief of e-Polymers journal and Chairman of the Editorial Board of the Polimery journal (Warsaw). He is also a member of the Editorial Boards of nine international journals, including Biomacromolecules, Journal of Polymer Science and Macromolecular Science. He worked at the Polymer Division of IUPAC as Titular Member, and in 2004 he was elected to the IUPAC Bureau. Besides, he chaired the World Polymer Congress in 2000, and in 1997–1999 he served as President of the European Polymer Federation. He has been awarded several prizes and medals including Palmes Academiques in France, Otto Warburg Prize in Germany and JASP Personal Medal in Japan.

Professor Penczek is an elected Member of the Polish Academy of Sciences, Doctor Honoris Causa of the Pierre et Marie Curie University in Paris and of the Russian Academy of Sciences. Recently he has been elected to the German Nordrhein Akademie der Wissenschaften.

A list of publications by Professor Stanisław Penczek is available at http://www.cbmm.lodz.pl/en/penczek.html

Piotr Petelenz

Professor of Theoretical Chemistry, Dr habil, PhD

Research profile

Excitons; Charge-transfer states; Polaritons; Vibronic coupling; Molecular aggregates; Electro-absorption spectra; Electrochromism

Post-doctoral Fellow (1977–78) and Visiting Professor (1986–88) at Queen's University, Kingston, Canada; Visiting Research Officer at National Research Council, Ottawa, Canada (1981, 1982, 1993); Visiting Professor at Ulm University, Germany (1983) and Université Louis Pasteur, Strasbourg, France (1985, 1990); Visiting Fellow in Research School of Chemistry, Australian National University, Canberra (1983); Lecturer (2001) at Fermi School of Physics, Varenna, Italy.

Current research focused on theoretical interpretation of electro-optical properties of organic solids, with special emphasis on the role of charge-transfer states, vibronic coupling and polaritonic effects. Recent accomplishment: a new approach to vibronic coupling in molecular crystals, with CT and Frenkel excitons treated on equal footing.

Selected publications

1. Bounds P.J., Siebrand W., Petelenz P., Charge transfer excitons in anthracene crystals. A theoretical investigation of their optical absorption and thermal dissociation, Chem. Phys., 63, 303–320, 1981.
2. Pac B., Petelenz P., Slawik M., Munn R.W., Theoretical interpretation of the electro-absorption spectrum of fullerene films, J. Chem. Phys., 109, 7932–7939, 1998.
3. Andrzejak M., Petelenz P., Slawik M., Munn R.W., Theoretical calculations of the electroabsorption spectrum of the sexithiophene single crystal, J. Chem. Phys., 117, 1328–1335, 2002.
4. Mazur G., Petelenz P., Slawik M., Theoretical calculations of the electroabsorption spectra of perylenetetracarboxylic dianhydride, J. Chem. Phys., 118, 1423–1432, 2003.
5. Eilmes A., Pac B., Petelenz P., Effect of the off-diagonal disorder on second-harmonic generation intensity in C_{60}, J. Lumin., 112, 295–298, 2005.
6. Petelenz P., Stradomska A., Theoretical interpretation of electro-absorption spectra for intense optical transitions, Phys. Rev., B71, 235205, 2005.
7. Broclawik E., Góra A., Liguzinski P., Petelenz P., Witek H.A., Quantum chemical modelling of electrochromism of tungsten oxide films, J. Chem. Phys., 124, 054709, 2006.
8. Stradomska A., Petelenz P., Electroabsorption spectra of linear porphyrin arrays – a model study, Mol. Phys., 104, 2063–2071, 2006.
9. Stradomska A., Petelenz P., Polariton effects in electroabsorption spectra of molecular crystals with several molecules in the unit cell – sexithiophene, Org. Electronics, 7, 551–561, 2006.
10. Zapotoczny S., Rymarczyk-Machał M., Stradomska A., Petelenz P., Nowakowska M., Aggregates of naphthalene chromophores in poly(vinylalcohol)-graft-poly(vinylnaphthalene) pseudomicelles, J. Phys. Chem. B, 111, 10088–10094, 2007.

Wojciech Piekoszewski

Professor of Medical Sciences, Dr habil, PhD

Research profile

Toxicology; Pharmacokinetics; Addictive substances; Alternative materials

European Registered Toxicologist; Head of the Polish Pharmaceutical Society, Kraków Branch (1995–1998); Head of the Polish Toxicological Society, Kraków Branch (2002–2008); Head of the Standing Committee of Working Group of the European Network of Forensic Science Institutes, The Hague, the Netherlands (2004–2005); Abstract Editor of Bulletin of the International Association of Forensic Toxicologists; Research Director of the Institute of Forensic Research (1997––2007).

Major scientific interest: determination of drugs of abuse in biological materials; application of alternative materials in toxicological analysis; methadone; buprenorfina and maintenance program; driving under the influence of alcohol and drugs; effects of tobacco smoke on the pregnant woman and foetus; genotoxic effects of tobacco smoke and drugs; biochemical effects of tobacco smoke; influence of tobacco smoke and alcohol on drugs pharmacokinetics; biomarkers of tobacco exposition; determination of tobacco specific carcinogens in biological fluids; disturbance of metals homeostasis in cancer patients.

Selected publications

1. Florek E., Ignatowicz E., Wrzosek J., Piekoszewski W., Effect of rutin on total antioxidant status of rats exposed to cigarette smoke, Pharmacol. Rep., 57, 84–89, 2005.
2. Scisłowski M., Piekoszewski W., Kamenczak A., Florek E., Simultaneous determination of buprenorphine and norbuprenorphine in serum by high-performance liquid chromatography-electrospray ionization-mass spectrometry, J. Anal. Toxicol., 29, 249–253, 2005.
3. Wilimowska J., Piekoszewski W., Krzyżanowska-Kierepka E., Florek E., Monitoring of verapamil enantiomers concentration in overdose – case report, Clin. Toxicol., 44, 169–171, 2005.
4. Węgrzyn P., Jura J., Kupiec T., Piekoszewski W., Władyka B., Zarębski A., Koj A., A search for genes modulated by interleukin-6 alone or with interleukin-1b cells using differential display analysis, Bichim. Biophys. Acta-Mol. Basis Dis., 1762, 319–328, 2006.
5. Wilimowska J., Florek E., Piekoszewski W., Disposition of valproic acid in self-poisoned adults, Basic Clin. Pharmacol. Toxicol., 99, 22–26, 2006.
6. Florek E., Piekoszewski W., Hubert A., Kornacka M.K., Active and passive smoking during pregnancy on newborn health, in: Jeffries T.C. (Ed.), Nova Science, Hauppauge NY USA, 2007, chapter IX, pp. 193–239.
7. Florek E., Piekoszewski W., Kulza M, Szindżikaszwili T., Gomółka E., Chuchraki M., Sędziak A., Interaction between tobacco smoking and alcohol in animal models. Pharmacol. Rep., 60, 985–990, 2008.

Leonard Marian Proniewicz

Professor of Chemistry, Dr habil, PhD

Research profile

Chemical physics; Studies of molecular structures; Raman, infrared and nuclear magnetic resonance spectroscopies; X-ray diffraction; Quantum-chemical calculations

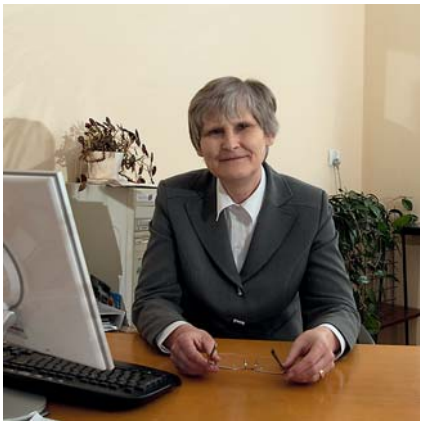
Our research focuses on the application of molecular spectroscopy, diffraction methods, and theoretical calculations to study structures of biologically active molecules and their model compounds.

Selected publications

1. Podstawka E., Proniewicz L.M., The orientation of BN-related peptides adsorbed on SERS-active silver nanoparticles: Comparison with a silver electrode surface, J. Phys. Chem. B, 113, 4978–4985, 2009.
2. Małek K., Podstawka E., Milecki J., Schroeder G., Proniewicz L.M., Structural features of the adenosine conjucate in means of vibrational spectroscopy and DFT, Biophys. Chem., 142, 17–26, 2009.
3. Helios K., Wysokiński J., Zierkiewicz W., Proniewicz L.M., Michalska D., Unusual noncovalent interaction between the chelated Cu(II) ion and π-bond in the vitamin B_{13} complex, *cis*-ammine(orotato)copper(II): theoretical and vibrational spectroscopy studies, J. Phys. Chem. B, in press.
4. Podstawka E., Ozaki Y., Proniewicz L.M., Structures and bonding on colloidal silver surface of the various length carboxyl terminal fragments of bombesin, Langmuir, 24, 10807–10816, 2008.
5. Kaczor A., Proniewicz L.M., Almeida R., Gomez-Zavaglia A., Cristiano M.L.S., Beja A.M.M., Silva M.R., Fausto R., The Chapman-type rearrangement in pseudosaccharins: The case of 3-(methoxy)-1,2-benzisothiazole 1,1-dioxide, J. Mol. Struct., 892, 343–352, 2008.
6. Podstawka E., Kafarski P., Proniewicz L.M., Structural properties of L-X-L-Met-L-Ala phosphonate tripeptides: A combined FT-IR, FT-RS, and SERS spectroscopy studies and DFT calculations, J. Phys. Chem. A, 112, 11744–11755, 2008.
7. Zborowski K., Proniewicz L.M., Theoretical studies on aromaticity of selected hydroxypyrones and their cations and anions. Part 2. Electron delocalization in the OCCO group, J. Phys. Org. Chem., 21, 207–214, 2008.
8. Małek K., Zborowski K., Gębski K., Proniewicz L.M., Schroeder G., 1,3,4-oxadiazoles: evaluation of aromaticity and atomic charge distribution, Mol. Phys., 106, 1823–1833, 2008.
9. Podstawka E., Andrzejak M., Kafarski P., Proniewicz L.M., Comparison of adsorption mechanism on colloidal silver surface of alafosfalin and its analogs, J. Raman Spectrosc., 39, 1238–1249, 2008.
10. Barańska M., Proniewicz L.M., Raman mapping of caffeine alkaloid, Vib. Spectrosc., 48,153–157, 2008.
11. Chruszcz-Lipska K., Barańska M., Proniewicz L.M., H-1 and C-13 NMR spectroscopy of structural isomers of pyridinephosphonic acids, J. Mol. Struct., 876, 278–287, 2008.

Barbara Rys

Dr habil, PhD



Research profile

Organic chemistry; Stereochemistry; Conformational analysis; Medium-sized rings; NMR

Our main interest is in the relationship between the conformation and the properties of organic compounds. We study the conformation of heterocyclic molecules possessing medium-sized rings with various functionalities in order to find the factors, both steric and stereoelectronic, determining ground-state geometry of the molecules. We use nuclear magnetic resonance spectroscopy and computational methods to examine conformation and conformational processes.

Selected publications

1. Bogdanowicz-Szwed K., Grochowski J., Obara A., Rys B., Serda P., Stereoselective synthesis of bridged azepine derivatives *via* polyfunctionalized spiro-annulated thiophene. Novel rearrangement of oxime esters, J. Org. Chem., 66, 7205–7208, 2001.
2. Karolak-Wojciechowska J., Czylkowski R., Karczmarzyk Z., Paluchowska M.H., Rys B., Szneler E., Mokrosz M.J, Structures and conformations of 1-aryl-1,4-dihydro-3(*2H*)-isoquinolinones, J. Mol. Struct., 612, 39–47, 2002.
3. Migda W., Rys B., GIAO/DFT evaluation of ^{13}C NMR chemical shifts of selected acetals based on DFT optimized geometries, Magn. Reson. Chem., 42, 459–466, 2004.
4. Migda W., Rys B., Conformational analysis of nine-membered cyclic acetals. Stereoelectronic effect in 2,4- and 3,5-benzodioxonine derivatives, J. Org. Chem., 71, 5498–5506, 2006.
5. Gomez E.D., Antus S., Ferenczi R., Rys B., Stankiewicz A., Duddeck H., Enantiodifferentiation by ^{1}H NMR spectroscopy (dirhodium method) – selectivity of oxygen functionalities, Nat. Prod. Commun., 3, 339–344, 2008.

Janusz J. Sepioł

Associate Professor of Chemistry, Dr habil, PhD

Research profile

Chemistry of alkylidene- and arylidene-malonodinitriles; Aromatic rearrangements; Chemistry of aromatic systems

Born 16 April 1946; PhD, 1974; Habilitation, 1987. Research interests of our group concentrate on syntheses of aromatic carbocyclic systems from acyclic precursors. A variety of alkylidene-, arylidenemalonodinitriles, and aryl-alkylidenecyanoesters has been cyclised to aromatic amino-nitriles and amino-esters. By this new annulation approach a convenient synthesis of benzo- and naphtho-fused cycloalkenes and also of alkyl-substituted benzenes and naphthalenes can be carried out. In the course of these investigations an interesting rearrangement of a carbocyclic framework of ylidenemalonodinitriles has been noticed.

Selected publications

1. Sepioł J.J., Góra M., Łuczyński M.K., Synthesis of cycloalka[a]- and cycloalka[c]phenanthrene aminonitriles from 2-(1-naphthyl)cycloalkylidene malonodinitriles involving novel aromatic rearrangement, Synlett., (9), 1383–1386, 2001.
2. Sepioł J.J., Wilamowski J., New aromatic rearrangement accompanying ring closure of A2-arylpropylidene-malonodinitriles to 1-aminonaphthalene-2-carbonitriles, Tetrahedron Lett., 42, 5287–5291, 2001.
3. Kozik B., Wilamowski J., Góra M., Sepioł J.J., Novel synthesis of α-arylnaphthalenes from diphenylacetaldehydes and 1,1-diphenylacetones, Tetrahedron Lett., 47, 3435–3438, 2006.
4. Kozik B., Wilamowski J., Góra M., Sepioł J.J., Synthesis of α-arylnaphthalenes from diphenylacetaldehydes and 1,1-diphenylacetones, Tetrahedron, 64, 6452–6460, 2008.

Barbara Sieklucka

Professor of Chemistry, Dr habil, PhD

Research profile

Coordination chemistry; Polynuclear coordination compounds; Inorganic molecular materials; Molecular magnetic materials

Current research activities are focussed on the development of new polynuclear coordination framework materials based on octacyanometalate $[M(CN)_8]^{3-/4-}$ (M = Nb, Mo, and W) building blocks and complexes of 3d (Mn, Fe, Co, Ni, Cu) and 4f (Ln=Ce-Lu excluding Pm) metal centres. The research includes the design, synthesis and the structural, spectroscopic and magnetic characterization of the hybrid inorganic-organic coordination networks. The networks represent functional materials, which is due to their broad structural and chemical diversity and to the potential of rational tuning of their properties, such as storage, exchange, magnetic and optical.

Bibliographic data: 71 publications in peer reviewed journals (up to 2008); 453 citations; h-index 11; Total Impact Factor = 148.07; 26 research grants.

Current international co-operation: Dr. Corine Mathoniere and Dr. Cedric Desplanches, l'Université de Bordeaux-1, Institut de Chimie de la Matière Condensée de Bordeaux, France; Prof. Andrea Caneschi, Laboratory of Molecular Magnetism, Dipartimento di Chimica e UdR INSTM di Firenze, Italy.

Selected publications

1. Mathoniere C., Podgajny R., Guionneau P., Labrugere Ch., Sieklucka B., Chem. Mater., 17, 442–449, 2005.
2. Sieklucka B., Podgajny R., Przychodzeń P., Korzeniak T., Coordin. Chem. Rev., 249, 2203–2221, 2005.
3. Korzeniak T., Stadnicka K., Pełka R., Bałanda M., Tomala K., Kowalski K. Sieklucka B., Chem. Commun., 2939–2941, 2005.
4. Przychodzeń P., Korzeniak T., Podgajny R., Sieklucka B., Coordin. Chem. Rev., 250, 2234–2260, 2006.
5. Podgajny R., Chmel N.P., Bałanda M., Tracz P., Gaweł B., Zając D., Sikora M., Kapusta C., Łasocha W., Wasiutyński T., Sieklucka B., J. Mater. Chem., 17, 3308–3314, 2007.
6. Nowicka B., Rams M., Stadnicka K., Sieklucka B., Inorg. Chem., 46, 8123–8125, 2007.
7. Podgajny R., Pinkowicz D., Korzeniak T., Nitek W., Rams M., Sieklucka B., Inorg. Chem., 46, 10416–10425, 2007.
8. Podgajny R., Nitek W., Rams M., Sieklucka B., Cryst. Growth Des., 8, 3817–3821,2008.
9. Pinkowicz D., Podgajny R., Bałanda M., Makarewicz M., Gaweł B., Łasocha W., Sieklucka B., Inorg. Chem., 47, 9745–9747, 2008.
10. Korzeniak T., Podgajny R., Gimenez-Saiz C., Stadnicka K., Rams M., Sieklucka B., Inorg. Chem., 2009, DOI: 10.1021/ic801989b.

Zbigniew Sojka

Professor of Chemistry, Dr habil, PhD

Research profile

Solid state and interfacial chemistry; Inorganic nanomaterials; Catalysis; Spectroscopy; Molecular modeling; Electron Magnetic Resonance Techniques

Appointments: Vice-Dean for Research and Cooperation; Head of the Inorganic Chemistry Department; Head of the Catalysis and Solid State Group; Head of the Faculty EPR Laboratory; Visiting Professor at the Universities of Paris and Lille.

The research interest of our group focuses on molecular design, spectroscopic characterization and reactivity studies of nanostructured, porous and bulk inorganic materials functionalized with transition metal ions. The functionalization aims at imparting desired properties to the investigated materials and at guiding surface reactions along specific pathways. In our methodology we use computational spectroscopy and molecular modeling for establishing quantitative structure-property-function relationships, and for working back from the observed kinetics to the underlying reaction mechanisms with quantum-atomistic resolution. Special emphasis is put on the elucidation of the electronic and magnetic structure of active sites and intermediates, and on the development and application of advanced EPR methods for in situ investigation of heterogeneous materials.

Selected publications

1. Spałek T., Pietrzyk P., Sojka Z., Application of genetic algorithm joint with Powell method to non-linear least-squares fitting of powder EPR spectra, J. Chem. Inf. Model., 45, 18–29, 2005.
2. Pietrzyk P., Sojka Z., Relativistic density functional calculation of EPR g tensor for the $\eta^1\{CuNO\}^{11}$ species in discrete and zeolite-embedded states, J. Phys. Chem. A, 109, 10571–10581, 2005.
3. Chiesa M., Giamello E., Di Valentin C., Paccioni G., Sojka Z., Van Doorslaer S., Nature of the chemical bond between metal atoms and oxide surfaces: New evidences from spin density studies of K atoms on alkaline earth oxides, J. Am. Chem. Soc., 127, 16935–16944, 2005.
4. Dablemont C., Hamaker C.G., Thouvenot R., Sojka Z., Che M., Maatta E.A., Proust A., Functionalization of heteropolyanions-osmium and rhenium nitrido derivatives of Keggin- and Dawson-type polyoxotungstates: Synthesis, characterization and multinuclear (^{183}W, ^{15}N) NMR, EPR, IR and UV/Vis fingerprints, Chem. Eur. J., 12, 9150–9160, 2006.
5. Kotarba A., Rożek W., Serafin I., Sojka Z., Reverse effect of doping on stability of principal components of styrene catalyst: $KFeO_2$ and $K_2Fe_{22}O_{34}$, J. Catal., 247, 238–244, 2007.
6. Pietrzyk P., Sojka Z., Dźwigaj S., Che M., Generation, identification, and reactivity of paramagnetic VO_2 centers in zeolite BEA for model studies of processes involving spin pairing, electron transfer, and oxygen transfer, J. Am. Chem. Soc., 129, 14174–14175, 2007.
7. Spałek T., Kruczała K., Sojka Z., Schlick S., Deducing 1D concentration profiles from EPR imaging: A new approach based on the concept of virtual components and optimization with the genetic algorithm, J. Magn. Reson., 189, 139–150, 2007.

Katarzyna M. Stadnicka

Professor of Chemistry, Dr habil, PhD

Research profile

Crystallography; Crystal chemistry; Crystal physics; Crystal engineering; X-ray structure analysis; Experimental charge density

Research areas: Structural aspects of physical, chemical and biological properties: crystal structure analysis, experimental charge density, crystal engineering, molecular packing; Intermolecular interactions, structure-property relationship for linear (OA, birefringence) and non-linear (SHG) optical properties; Structural mechanisms of phase transitions; Structure-pharmacological activity relationship for compounds showing antiarrhythmic and/or adrenergetic properties; Structure of minerals (blue halite).

Research associates and their topics: Anna Krawczuk – Chirality of crystals in the view of optical activity and experimental charge density studies; Alicja Janik – Interactions between antiarrhythmic agents and ion channels using diffraction methods, NMR spectroscopy and molecular modeling; Marlena Gryl – Crystal engineering of materials with potential non-linear optical properties; Marzena Suder – Cells interactions with the mineral apatite plates of known crystallographic orientation; Sylwia Zelek – Structure-property relationship in blue halite from Kłodawa Salt Mine.

Selected publications

1. Hryniewicz K., Stadnicka K., Pattek-Janczyk A., J. Mol. Struct., 919, 255–270, 2009.
2. Janik A., Olech A., Stasiewicz-Urban A., Stadnicka K., Acta Crystalogr. C, 65, o70–o75, 2009.
3. Gryl M., Krawczuk A., Stadnicka K., Acta Crystalogr. B, 64, 623–632, 2008.
4. Trzewik B., Cież D., Hodorowicz M., Stadnicka K., Synthesis, 18, 2977–2985, 2008.
5. Zelek S., Stadnicka K., Szklarzewicz J., Natkaniec-Nowak L., Toboła T., Miner. Resour. Manage., 24, 159–172, 2008.
6. Janik A., Jarocha M., Stadnicka K., Acta Crystalogr. B, 64, 223–229, 2008.
7. Budzowski A., Pitak M., Stadnicka K., Monatsh. Chem., 138, 1257–1266, 2007.
8. Matoga D., Szklarzewicz J., Stadnicka K., Shongwe M.S., Inorg. Chem., 46, 9042–9044, 2007.
9. Janik A., Chyra A., Stadnicka K., Acta Crystalogr. C, 63, o572–o575, 2007.
10. Galuskin E.V., Galuskina I.O., Stadnicka K., Armbruster T., Kozanecki M., Can. Mineral., 45, 239–248, 2007.
11. Krawczuk A., Stadnicka K., Acta Crystalogr. C, 63, m448–m450, 2007.
12. Nowicka B., Rams M., Stadnicka K., Sieklucka B., Inorg. Chem., 46, 8123–8125, 2007.
13. Flakus H.T., Śmiszek-Lindert W., Stadnicka K., Chem. Phys., 335, 221–232, 2007.
14. Wojtas Ł., Pawlica D., Stadnicka K., J. Mol. Struct., 785, 14–20, 2006.

Grażyna Stochel

Professor of Chemistry, Dr habil, PhD

Research profile

Inorganic and Bioinorganic Chemistry; Photochemistry and Photophysics; Nanochemistry and Nanotechnology

Humboldt Fellow at the Universities of Frankfurt/Main, Regensburg and Erlangen-Nürnberg; Visiting Researcher at the Universities of Ferrara, Padova, Barcelona, Orleans, Lund, and Coimbra; Head of the Coordination and Bioinorganic Physicochemistry group.

Research activity is focused on: (i) mechanisms of inorganic and bioinorganic reactions, (ii) high pressure kinetic techniques, (iii) photochemistry and photophysics of coordination compounds, (iv) photocatalysis, (v) metal compounds, small molecules and light in biology, environment and medicine, and (vi) nanochemistry and functional materials. Scientific expertise and modern equipment available in the group include spectroscopic, kinetic, photochemical, electrochemical, microscopic and some biochemical techniques. The group is involved in various international and national research projects in the Bio-Techno area. Interesting and up-to-date subjects, their applications with theoretical background, interdisciplinarity and internationalisation are the most important determinants for our research activity.

More information: www.bioinorg.nanophotonics.pl

Selected publications

1. Stochel G., Stasicka Z., Brindell M., Macyk M., Szaciłowski K., Bioinorganic Photochemistry, 398 pages, Wiley, 2009.
2. Orzeł Ł., Fiedor L., Kania A., Wolak M., van Eldik R., Stochel G., Interplay between acetate ions, the peripheral groups, and the reactivity of the core nitrogens in transmetalation of tetrapyrroles, Chem. Eur. J., 14, 9419–9430, 2008.
3. Mitoraj D., Jańczyk A., Strus M., Kisch H., Stochel G., Heczko P.B., Macyk W., Visible light inactivation of bacteria and fungi by modified titanium dioxide, Photochem. Photobiol. Sci., 6**,** 642–648, 2007.
4. Brindell M., Kuliś E., Elmroth S.K.C., Urbanska K., Stochel G., Light-Induced anticancer activity of $[RuCl_2(DMSO)_4]$ complexes, J. Med. Chem., 48, 7298–7304, 2005.
5. Macyk W., Franke A., Stochel G., Metal compounds and small molecules activation – case studies, Coord. Chem. Rev., 249, 2437–2457, 2005.
6. Szaciłowski K., Macyk W., Drzewiecka-Matuszek A., Brindell M., Stochel G., Bioinorganic photochemistry. Frontiers and mechanisms, Chem. Rev., 105, 2647–2694, 2005.
7. Wanat A., Wolak M., Orzeł Ł., Brindell M., van Eldik R., Stochel G., Laser flash photolysis as tool in the elucidating of the nitric oxide binding mechanism to metallobiomolecules, Coord. Chem. Rev., 229, 37–49, 2002.
8. Laverman L.E., Wanat A., Oszajca J., Stochel G., Ford P., van Eldik R., Mechanistic studies on the reversible binding of nitric oxide to metmyoglobin, J. Am. Chem. Soc., 123**,** 285–293, 2001.

Konrad Szaciłowski

Dr habil, PhD

Research profile

Semiconducting materials; Molecular scale devices; Nanoelectronics; Optoelectronics

Konrad Szaciłowski was born in Kraków, Poland in 1971. He graduated from the Jagiellonian University in 1995 (MSc in cooperation with Professor Horst Kisch, Erlangen, Germany) and in 2000 he completed his PhD under the guidance of Professor Zofia Stasicka. As a postdoc fellow he worked for one year with Professor John F. Endicott (Wayne State University) on synthesis, spectroscopy, magnetic properties and electrochemistry of nickel complexes with macrocyclic ligands. Presently he is a member of the Coordination and Bioinorganic Physicochemistry group, of the Centre for Inorganic Nanochemistry "nanoInchem" and of the Molecular Nanoelectronics Research Network "NanoMol". His research interests are focused mainly on surface engineering of nanocrystalline materials, microwave-assisted synthesis and (photo)electrochemistry of wide band gap semiconductors, information processing at molecular level and molecular nanoelectronics. Furthermore, he recently got involved in detailed spectroscopic investigations of doped chalcogenide semiconductors and quantum-chemical modelling of semiconductor nanoparticles.

Selected publications

1. Szaciłowski K., Macyk W., Stochel G., Light-driven OR and XOR programmable chemical logic gates, J. Am. Chem. Soc., 128, 4550–4551, 2006.
2. Szaciłowski K., Macyk W., Working prototype of an optoelectronic XOR/OR/YES reconfigurable logic device based on nanocrystalline semiconductors, Solid State Electron., 50, 1649–1655, 2006.
3. Szaciłowski K., Macyk W., Hebda M., Stochel G., Redox-controlled photosensitization of nanocrystalline titanium dioxide, ChemPhysChem., 7, 2384–2391, 2006.
4. Szaciłowski K., Macyk W., Stochel G., Synthesis, structure and photoelectrochemical properties of the TiO_2 – Prussian blue nanocomposite, J. Mater. Chem., 16, 4603–4611, 2006.
5. Macyk W., Stochel G., Szaciłowski K., Photosensitization and photocurrent switching effect in nanocrystalline titanium dioxide functionalized with iron(II) complexes: A comparative study, Chem. Eur. J., 13, 5676–5687, 2007.
6. Gawęda S., Stochel G., Szaciłowski K., Bioinspired nanodevice based on the folic acid − titanium dioxide system, Chem. Asian J., 2, 580–590, 2007.
7. Szaciłowski K., Biomedical implications of information processing in chemical systems: Non-classical approach to photochemistry of coordination compounds, BioSystems, 90, 738–749, 2007.
8. Szaciłowski K., Digital information processing in molecular systems, Chem. Rev., 108, 3481–3548, 2008.
9. Gawęda S., Stochel G., Szaciłowski K., Photosensitization and photocurrent switching in carminic acid/titanium dioxide hybrid material, J. Phys. Chem. C, 112, 19131–19141, 2008.

Janusz Szklarzewicz

Dr habil, PhD

Research profile

Inorganic chemistry; Complexes; Transition metals; Reaction mechanisms; Ligand activation; Catalysis

Professor J. Szklarzewicz is Head of the Coordination Chemistry group in the Department of Inorganic Chemistry. The principal aim of research in the group is the detailed experimental investigation of the structure and properties of metal complexes. This includes the isolation of new compounds with rare coordination numbers and/or symmetry, and the investigation of the kinetics and mechanisms of complex formation. Other research topics include activation of small molecules, metal assisted catalysis and ligand activation, the latter being of special importance in that it provides information on the production of new organic molecules in simple one step reactions in aqueous solutions. We also study the metal complexes as a possible means of modification of surface properties, for instance through deposition of nanolayers on metal surfaces, and as pharmaceutics. In this last topic complexes of insulin mimetic properties are studied.

Selected publications

1. Matoga D., Szklarzewicz J., Lewiński K., Cyanooxo molybdenum(IV) complex with 2-pyrazinecarbonitrile and 2-pyrazinecarboxylate: crystallographic and spectroscopic studies reveal metal-assisted nitrile hydrolysis, Polyhedron, 27, 2643–2649, 2008.
2. Szklarzewicz J., Matoga D., Kłyś A., Łasocha W., Ligand-field photolysis of $[Mo(CN)_8]^{4-}$ in aqueous hydrazine: trapped Mo(II) intermediate and catalytic disproportionation of hydrazine by cyano-ligated Mo(III,IV) complexes, Inorg. Chem., 47, 5464–5472, 2008.
3. Szklarzewicz J., Matoga D., Niezgoda A., Yoshioka Y., Mikuriya M., Missing link in the ligand-field photolysis of $[Mo(CN)_8]^{4-}$: synthesis, X-ray crystal structure and physicochemical properties of $[Mo(CN)_6]^{2-}$, Inog. Chem., 46, 9531–9533, 2007.
4. Matoga D., Szklarzewicz J., Stadnicka K., Shongwe M.S., Iron(III) complexes with a biologically relevant arylhydrazone: crystallographic evidence for coordination versatility, Inorg. Chem., 46, 9042–9044, 2007.
5. Stawski T., Szklarzewicz J., Kotarba A., Stelmachowski P., The modifications of copper work function by layer-by-layer deposition of $[W(CN)_8]^{4-}$ – Co^{2+} bimetallic nanolayers, Polyhedron, 28, 473–478, 2009.
6. Matoga D., Mikuriya M., Szklarzewicz J., $(PPh_4)_3[W(CN)_7(O_2)]\cdot 4H_2O$ as the representative of the $[M(L)_7(LL)]$ class for nine-coordinate complexes, Inorg. Chem., 45, 7100–7104, 2006.
7. Matoga D., Mikuriya M., Handa M., Szklarzewicz J., Self-assembly of mixed-valent ruthenium(II,III) pivalate and octacyanotungstate(V) building blocks, Chem. Lett., 34, 1550–1551, 2005.
8. Matoga D., Szklarzewicz J., Fawcett J., Unexpected direct incorporation of NO in the Mo(IV) coordination sphere. X-ray crystal structure of $(PPh_4)_4[\{Mo(CN)_5(NO)\}2(\mu\text{-pz})]\cdot 2C_2H_5OC_2H_5$, Polyhedron., 24, 1533–1539, 2005.

Andrzej M. Turek

Dr habil, PhD

Research profile

Photochemical synthesis of vitamin D; Cis-trans photoisomerization; Principal component analysis

We aim to elucidate the mechanisms of selected photochemical reactions by chemical and spectroscopic means. We are guided by the premise that a detailed understanding of simple photochemical reactions establishes the proper foundation for the study of more complex photochemical and photobiological systems. Our methods include quantitative measurements of product quantum yields, determination of rate constants by employing steady-state and transient emission and absorption spectroscopy, use of triplet excitation transfer to sensitize or quench triplet reaction pathways. An important goal is the integration of all the information into a self-consistent kinetics model for each reaction. We also study the effects of medium and temperature on the photochemical and photophysical events. For that we proposed a new method of compensation for thermal broadening in the electronic absorption and fluorescence spectra which significantly facilitates the resolution of the spectral matrices into the spectral contributions from pure components. Most of this research is a result of successful collaboration with a photochemical research group guided by Professor Jack Saltiel at the Florida State University, Tallahassee, FA.

One specific topic of our research is the elucidation of the pathways that lead to the cis-trans photoisomerization of olefins. We have developed the method of principal component analysis with self-modeling (PCA-SM) to resolve the spectra of such systems into the separate contributions from distinct conformers. Another topic is the light-induced reactions that lead to the formation of vitamin D in the skin and in industrial reactions. We have developed an enhanced method of photochemical synthesis of vitamin Ds. Our method includes irradiating a reaction mixture of precursor molecules with light at 254 and 313 nm to produce previtamin D, and heating at a temperature not exceeding 100 °C to convert previtamin D to vitamin D.

Selected publications

1. Saltiel J., Sears D.F., Jr., Turek A.M., J. Phys. Chem. A, 105, 7569–7578, 2001.
2. Turek A.M., Krishnamoorty G., Phipps K., Saltiel J., J. Phys. Chem. A, 106, 6044–6052, 2002.
3. Saltiel J., Cires L., Turek A.M., J. Am. Chem. Soc., 125, 2866–2867, 2003.
4. Saltiel J., Cires L., Turek A.M., Conformer specific photochemistry in the vitamin D field, in: Handbook of Organic Photochemistry and Photobiology, Horspool W.M., Lenci F. (Eds), CRC Press, London, 2nd Ed., pp. 27-1–27-22, 2004.
5. Turek A.M., Krishnamoorthy G., Sears D.F., Jr., Garcia I., Dmitrenko O., Saltiel J., J. Phys. Chem. A, 109, 293–303, 2005.
6. Saltiel J., Krishna T.R.S., Turek A.M., J. Am. Chem. Soc., 127, 6938–6939, 2005.
7. Saltiel J., Krishna T.R.S., Turek A.M., Clark R.J., Chem. Commun., (14) 1506–1508, 2006.

Aleksandra Wesełucha-Birczyńska

Dr habil, PhD

Research profile

Transition metal chemistry; Drugs: antimalarials, antineoplastics, aneasthetics; Catalysts; Minerals and biominerals; Biopolymers; Infrared, Raman, resonance Raman and EPR spectroscopy; Mapping and imaging; 2D correlation analysis

The focus of research is on understanding the molecular structure of selected drugs, their aggregation capabilities and interactions with surrounding molecules, in addition to the consequent properties that include their transport through biological membranes and binding abilities. Spectroscopic and structural studies of a variety of transition-metal compounds have been performed to establish structure/spectroscopy relationships. By contrast, the characterization of selected minerals/biominerals and biopolymers by Raman microscopy and other techniques allowed us to account for the diversity observed in natural samples and also for their anisotropic spectroscopic properties.

Selected publications

1. Wesełucha-Birczyńska A., Proniewicz L.M., Bajdor K., Nakamoto K., Resonance Raman spectra of dioxygen adducts of manganese(II) porphyrins in dioxygen matrices, J. Raman Spectrosc., 22, 315–319, 1991.
2. Wesełucha-Birczyńska A., Nakamoto K., UV Resonance Raman studies on cinchonine polynucleotide interactions, J. Mol. Struct., 294, 127–130, 1993.
3. Wesełucha-Birczyńska A., Nakamoto K., Study of the interaction of the antimalarial drug cinchonine with nucleic acids by Raman spectroscopy, J. Raman Spectrosc., 27, 915–919, 1996.
4. Wesełucha-Birczyńska A., FT-Raman study of cinchonine aqueous solutions with varying pH; 2D correlation method, J. Mol. Struct., 480–481, 471–474, 1999.
5. Wesełucha-Birczyńska A., Strahan G.D., Tsuboi M., Nakamoto K., Interaction of bleomycin A_2 with DNA studied by resonance Raman spectroscopy: Intercalation or groove-binding, J. Raman Spectrosc., 31, 1073–1077, 2000.
6. Wesełucha-Birczyńska A., Oleksyn B.J., Hoffmann S.K., Śliwiński J., Borzęcka-Prokop B., Goslar J., Hilczer W., Flexibility of $CuCl_4$-tetrahedra in bis[cinchoninium tetrachlorocuprate(II)] trihydrate single crystals. X-ray diffraction and EPR studies, Inorg. Chem., 40, 4526–4533, 2001.
7. Wesełucha-Birczyńska A., 2D correlation method applied to FT-Raman investigations of cinchonidine aqueous solutions with varying pH, Vib. Spectrosc., 30, 77–83, 2002.
8. Wesełucha-Birczyńska A., Aggregation phenomena of cinchonine in aqueous solutions observed and analysed by 2D FT-Raman spectroscopy, Vib. Spectrosc., 35, 189–198, 2004.
9. Wesełucha-Birczyńska A., Toboła T., Natkaniec-Nowak L., Raman microscopy of inclusions in blue halites, Vib. Spectrosc., 48, 302–307, 2008.

Ewa Witek

Dr habil, PhD

Research profile

Polymers; Polyelectrolytes; Functional polymers

In her research activity, starting from the graduation at the Jagiellonian University, she focuses on the chemistry and technology of polymers. She works in the research group of Professor Edgar Bortel, since 1990s concentrating mainly on practical applications of water-soluble polymers, hydrogels and superabsorbents. She cooperates with the Faculties of Metallurgy and of Drilling, Oil and Gas of the AGH University of Science and Technology in Kraków, as well as with the Oil and Gas Institute in Kraków. As an academic teacher she teaches chemistry and technology of polymers. Since 2000 she is secretary of the Kraków Branch of the Polish Chemical Society.

Selected publications

1. Witek E., Kochanowski A., Bortel E., On the reaction of glycidol with a secondary amine, Macromol. Chem. Rapid Com., 21, 1108–1112, 2000.
2. Kochanowski A., Witek E., Bortel E., Wholly water-soluble interpolymer complexes formed by interaction of strong anionic and cationic polyelectrolytes, J. Macromol. Sci. A, 40, 449–460, 2003.
3. Witek E., Kochanowski A., Bortel E., Polielektrolity z merami winyloaminowymi i produkty ich modyfikacji, Przem. Chem., 82, 889–892, 2003.
4. Witek E., Kochanowski A., Bortel E., Nowy sposób syntezy hydrofobowo modyfikowanego poli(kwasu akrylowego), Polimery, 49, 3–8, 2004.
5. Bielewicz D., Witek E., Janota M., Knez D., Neue Konzepte der Synthese und Anwendung von amphoteren Polymeren in Bohrspülungen, Erdöl Erdgas Kohle, 120, 9–12, 2004.
6. Bortel E., Witek E., Kochanowski A., Pazdro M., Poliwinyloamina źródłem nowych możliwości rozwoju polimerów hydrofilowych, Polimery, 50, 491–500, 2005.
7. Witek E., Kochanowski A., Pazdro M., Bortel E., Mikroemulsje jako źródło nanolateksów i nanoreaktorów, Polimery, 51, 507–516, 2006.
8. Witek E., Pazdro M., Bortel E., Mechanism for base hydrolysis of poly(N-vinylformamide), J. Macromol. Sci. A, 44, 503– 507, 2007.
9. Bortel E., Witek E., Pazdro M., Kochanowski A., N-winyloformamid – nowy ekologiczny monomer wodorozpuszczalny, Polimery, 52, 503–510, 2007.
10. Witek E., Crosslinking copolymerization of N-vinylformamide in inverse suspension, Polimery, 53, 477–480, 2008.

Marek Janusz Wójcik

Professor of Chemistry, Dr habil, PhD

Research profile

Physical and theoretical chemistry; Molecular spectroscopy; Hydrogen bonded systems

Degrees in chemistry: MSc with honours 1968; PhD 1973; habilitation 1980, all at the Jagiellonian University; Professor of Chemistry 1996.

Appointments: Jagiellonian University (since 1968); Head of the Laboratory of Molecular Spectroscopy (since 1981); Professor extraordinary (1996–2003), Professor ordinary (since 2003). *Foreign experience*: Research Associate, NRC Canada (1977–78), JSPS Research Fellow, University of Tokyo (1982–83), Visiting Professor: University of Uppsala (1981, 1982, 1988–89), University of Chicago (1984–86), Oklahoma State University (1991–92), University of Illinois, Chicago (1982), Kyushu University (1995), IMS, Okazaki (1997–98), KEK, Tsukuba (2000–2002), University of Perpignan (2004), Kwansei Gakuin University (2007), Technical University of Munich (2007, 2008).

Research areas: (i) theoretical studies of hydrogen-bonded systems, water, aqueous ionic solutions, ices and molecules absorbed in ices, (ii) quantum-mechanical calculations, (iii) theoretical studies of multidimensional proton tunneling. *Research staff*: Marek Boczar, Dr habil, PhD, Dorota Jamróz, PhD, Łukasz Boda, PhD.

More information: www.chemia.uj.edu.pl/~wojcik

Selected publications

1. Wójcik M.J., Nakamura H., Iwata S., Tatara W., Theoretical study of multidimensional proton tunneling in the excited state of tropolone, J. Chem. Phys., 112, 6322–6328, 2000.
2. Wójcik M.J., Szczeponek K., Ikeda S., Theoretical study of the OH/OD stretching regions of the vibrational spectra of ice Ih, J. Chem. Phys., 117, 9850–9857, 2002.
3. Blaise P., Wójcik M.J., Henri-Rousseau O., Theoretical interpretation of the lineshape of the gaseous acetic acid dimer, J. Chem. Phys., 122, 064306, 2005.
4. Boczar M., Boda Ł., Wójcik M.J., Theoretical model for a tetrad of hydrogen bonds and its application to interpretation of infrared spectra of salicylic acid, J. Chem. Phys., 124, 084306, 2006.
5. Boczar M., Boda Ł., Wójcik M.J., Theoretical model of infrared spectra of hydrogen bonds in molecular crystals and its application to interpretation of infrared spectra of 1-methylthymine, J. Chem. Phys., 125, 084709, 2006.
6. Boczar M., Boda Ł., Wójcik M.J., Theoretical modeling of the O-H stretching IR bands of hydrogen-bonded dimers of benzoic acid in S_0 and S_1 electronic states, J. Chem. Phys., 127, 084307, 2007.
7. Boczar M., Kwiendacz J., Wójcik M.J., Theoretical and spectroscopic study of infrared spectra of hydrogen-bonded 1-methyluracil crystal and its deuterated derivative, J. Chem. Phys., 128, 164506, 2008.
8. Rekik N., Oujia B., Wójcik M.J., Theoretical infrared spectral density of H-bonds in liquid and gas phases: anharmonicities and dampings effects, Chem. Phys., 352, 65–76, 2008.

Szczepan Zapotoczny

Dr habil, PhD

Research profile

Nanotechnology; Photochemistry; Materials science; Surface chemistry; Self-assembled systems; Polymer brushes; Polymer films; Controlled radical polymerizations

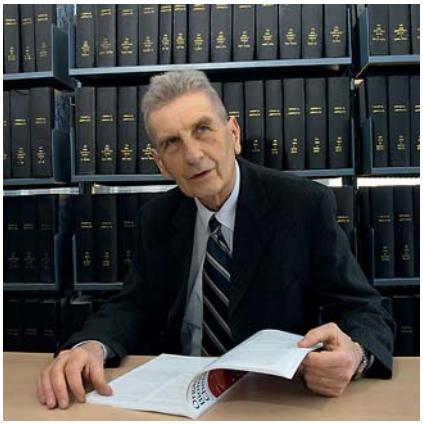
Szczepan Zapotoczny is head of *Nano-engineering of Functional Materials* team in *Nanotechnology of Polymers and Biomaterials* group and also chair of *Atomic Force Microscopy Laboratory.* His current research interests focus on nanostructural polymeric materials (films, brushes) for photochemical and biomedical applications as well as hybrid systems containing superparamagnetic and noble metal nanoparticles. The main techniques he develops is layer-by-layer (LbL) self-assembly of charged nanoobjects (polyelectrolytes, nanoparticles) and polymer brush synthesis using controlled radical polymerizations. The studied phenomena include photoinduced electron and energy transfer, stimuli-responsive behavior of "smart" polymers, controlled release of molecules from microparticles, and ligand-receptor interaction in biological systems.

His studies of soft matter are interdisciplinary and involve expertise from nanotechnology, materials science, biology and medicine. He cooperates with many national and foreign groups working on e.g. functional polymeric coatings for biological objects, stimuli responsive brushes or biological synthesis of silver nanoparticles.

Selected publications

1. Benetti E.M., Sui X., Zapotoczny S., Vancso G.J., Surface-grafted gel-brush/metal nanoparticle hybrids, Adv. Funct. Mat., 20, 939–944, 2010.
2. Bulwan M., Zapotoczny S., Nowakowska M., Robust one-component chitosan-based ultrathin films fabricated using layer-by-layer technique, Soft Matter, 5, 4726–4732, 2009.
3. de Klerk J., Bader A., Zapotoczny S., Sterzel M., Pilch M., Danel A., Gooijer C., Ariese F., Excited-state double proton transfer in 1H-pyrazolo[3,4-b]quinoline dimers, J. Phys. Chem. A, 113, 5273–5279, 2009.
4. Zapotoczny S., Golonka M., Nowakowska M., Nanostructured micellar films formed via layer-by-layer deposition of photoactive polymer, Langmuir 24, 5868–5876, 2008.
5. Zapotoczny S., Benetti E.M., Vancso G.J., Preparation and characterization of macromolecular "hedge" brushes grafted from Au nanowires, J. Mat. Chem. 17, 3293–3296, 2007.
6. Rymarczyk-Machał M., Zapotoczny S., Nowakowska M., Synthesis and characterization of novel photoactive polymer poly(vinyl alcohol)-graft-poly(vinyl naphthalene), J. Polym. Sci. A: Polym. Chem., 44, 2675–2683, 2006.
7. Zapotoczny S., Golonka M., Nowakowska M, Novel photoactive polymeric multilayer films formed via electrostatic self-assembly, Macromol. Rapid Commun., 26, 1049–1054, 2005.

Emeriti Professors



Andrzej Barański

Professor of Chemistry, Dr habil, PhD

Research Profile

Chemical kinetics; Catalysis; Degradation and de-acidification of paper

My research topics have included: properties of ammonia-CO_2-water system and synthesis of urea from CO_2 and ammonia (1955–1975), temperature programmed desorption from gas-solid ZnO-H_2 and zeolites-butenes systems (1970–1979), high-temperature oxidation of graphite electrodes (1982–1992), reduction of fused iron catalyst for ammonia synthesis – the bellwether reaction in heterogeneous catalysis (1967–2000), reduction of iron ores, mainly hematite to magnetite (1985–1997), and degradation and de-acidification of paper (1996 to present).

Stability of paper – an essential information carrier – is the main subject of my present research. Therein, the most significant scientific result is a mixed-control mechanism involving acid hydrolysis and oxidation proposed for the description of the kinetics of paper degradation [1]. More visibly, further to this research my activity included (i) participation in the task group for the elaboration of a long-term National Programme *Acid Paper*; (ii) implementation of the American *Bookkeeper III* technology in the Jagiellonian Library for the de-acidification of Polish book collections from the 19th and 20th century. The de-acidification has now reached a yield of ca. 30 tons of prints per year, and importantly, its implementation is a successful joint effort of people of sciences and humanities. Hopefully, such efforts will be conducive to the effective development of conservation chemistry in Poland [2].

My most recent field of interest is also the post Second World War history. An article based on the Barański family archives revealed the activities concerning the genesis of the European Union that up to now have been out of sight [3].

Author of over 100 publications and of three book chapters; Organizer and Head of the Regional Laboratory of Physicochemical Analyses and Structural Research (1972–1995); Plenipotentiary of the Rector of the Jagiellonian University for the Polish National Programme *Acid Paper* (2000–2008).

Selected publications

1. Barański A., Łagan J.M., Łojewski T., Acid catalysed degradation, in: Aging and Stabilisation of Paper, Strlič M., Kolar J. (Eds), University of Ljubljana, 2005, pp. 95–109.
2. Barański A., Chemia konserwatorska – podstawowe uwarunkowania jej rozwoju, Nauka i Zabytki, Muzeum Archeologiczne, Warszawa, 1**,** 7–11, 2008.
3. Barański A., Gdy ważyły się losy zjednoczenia Europy, Alma Mater, Jagiellonian University, Kraków, 98, 22–27, 2007.

Adam Bielański

Professor of Chemistry, Honorary Professor of the Jagiellonian University, PhD

Research profile

Solid state and physical chemistry; Heterogenous catalysis; Acid-base catalysis

Solid state chemistry: kinetics and mechanism of thermal decomposition (hydrated salts and hydroxides), polymorphic transformations (beryllates) and solid state reactions of spinels; Heterogenous catalysis and physical chemistry of transition metal oxides and polyoxometallates: electronic processes in catalysis on semiconducting oxides, physicochemical and catalytic properties of V_2O_5-MoO_3 system and catalytic oxidation processes; Acid-base type catalysis on zeolites and heteropolyacids.

Professor of physical and inorganic chemistry at AGH University of Science and Technology in Kraków, 1936–39, 1945–64; British Council scholar at Imperial College of Science and Technology, London, 1948–49; Head of Inorganic Chemistry Department, 1964–83; Vice-Rector of the Jagiellonian University, 1966–68; Professor at Institute of Catalysis and Surface Chemistry, Polish Academy of Sciences, 1983 to present.

Vice-President of the Polish Academy of Sciences, 1990–96, and of the Polish Academy of Arts and Sciences, 1990–94; Honorary doctorates from AGH University of Science and Technology and of Wrocław University; City of Kraków medal "Cracoviae Merenti".

Selected publications

1. Bielański A., Dereń J., Haber J., Słoczyński J., Electronic processes accompanying the catalytic dehydrogenation of alcohol on semiconducting oxide catalysts, Actes du Deuxième Congres International de la Catalyse 1960, Edition Technip, Paris, 1–26, 1961.
2. Bielański A., Some applications of electroconductivity measurement to the investigation of catalytic processes on semiconducting oxide catalysts, Catalysis and Chemical Kinetics, academic Press and WNT, New York–Warszawa, 93–128, 1964.
3. Bielański A., Najbar M., V_2O_5-MoO_3 catalysts for benzene oxidation, J. Appl. Catal. A, 157, 223–261, 1997.
4. Bielański A., Surface of transition metal oxides: concepts and ideas, in: Ceramic Interfaces: Properties and Applications, Smart R.S.C. and Nowotny J. (Eds.), IOM Communications Ltd. London, 16–30, 1998.
5. Małecka A., Poźniczek J., Micek-Ilnicka A., Bielański A.,Gas phase synthesis of MTBE on dodecatungstosilicic acid as the catalyst, J. Mol. Catal. A, 138, 67–81, 1999.
6. Bielański A., Lubańska A., FTIR investigation of Wells-Dawson and Keggin type heteropolyacids, J. Mol. Catal. A, 224, 179–187, 2004.
7. Bielański A., Małecki A., Lubańska A., Diemann E., Bogge H., Müller A., The behaviour of NH_4^+ in a water nanodrop encapsulated within a highly charged porous metal-oxide nanocontainer: A thermoanalytical study, Inorg. Chem. Commun., 11, 110–113, 2008.

Books

1. Bielański A., Podstawy Chemii Nieorganicznej, 5th ed, PWN, Warszawa, 520 pages, 2006.
2. Bielański A., Haber J., Oxygen in Catalysis, Marcel Dekker, New York, 472 pages, 1991.

Krystyna Bogdanowicz-Szwed

Professor of Chemistry, Dr habil, PhD

Research profile

Development of efficient synthetic methods of heterocyclic compounds by cyccloaddition and conjugate addition

MSc in chemistry, 1956, Jagiellonian University; PhD, 1962, Jagiellonian University (under supervision of Dozent Dr. J. Schoen); Habilitation, 1978, Jagiellonian University; Professor of the Jagiellonian University, 1991–1996; Full Professor, 1996, Visiting Professor at the University in Bochum, Germany (1982 and 1985) and at the University in Goettingen, Germany (1986 and 1992).

Head of research group, 1984–2004. The main subject of research concerns the synthesis of nitrogen, sulfur and oxygen heterocyclic compounds of potential biological activity and of analogues of some natural products.

1994–1998, Scientific cooperation with DuPont Agricultural Co. (USA),

2000–2004, Scientific cooperation with Taisho Pharmaceutical Co. (Japan).

The textbook "The Conservation of Orbital Symmetry in Pericyclic Reaction" by K. Bogdanowicz-Szwed and E. Śledziewska was awarded a prize by the Ministry of Education in 1981.

Supervisor of six PhD theses and numerous MSc works.

Selected publications

1. Bogdanowicz-Szwed K., Pałasz A., Polycyclic *2H*-pyran derivatives by intramolecular hetero-Diels-Alder reactions of α-sulfur-substituted α,β-unsaturated carbonyl compounds, Monatsh. Chem., 132, 393–401, 2001.
2. Bogdanowicz-Szwed K.,. Budzowski A., Efficient synthesis of functionalized 2*H*-thiopyrans *via* hetero-Diels-Alder reactions of an enaminothione with electrophilic olefins, Monatsh. Chem., 132, 947–957, 2001.
3. Bogdanowicz-Szwed K., Grochowski J., Obara A., Rys B., Serda P., Stereoselective synthesis of bridged azepine derivatives *via* polyfunctionalized spiroannulated thiophene. Novel rearrangement of oxime esters, J. Org. Chem., 66, 7205–7208, 2001.
4. Bogdanowicz-Szwed K., Budzowski A., Hetero-Diels-Alder reactions of enaminothione with electrophilic olefins. Synthesis of 2-furyl substituted *2H*-thiopyrans, Z. Naturforsch., 57 b, 637–642, 2002.

Edgar Bortel

Professor of Chemistry, Dr habil, PhD

Research profile

Chemical technology; Polymers

His scientific career started in 1951 when he became an assistant of Professor Feliks Polak, Head of the newly founded Department of Chemical Technology at the Jagiellonian University. From the beginning his interests were devoted to synthetic polymers, a quickly developing field of research at those days. In his PhD (1959) and habilitation (1968) theses he dealt with synthesis and physicochemical characterization of ion-exchange resins. In 1970 he set up a research group working on preparation, characterization and practical applications of polymers, mainly those suitable for flocculation of coal-muds, also additives in drilling muds and foamers in copper-dressing. For his scientific achievements he has been granted awards by the Secretary of the Polish Academy of Sciences, by the Minister of Heavy Industry, and the Rectors of the Jagiellonian and AGH Technical Universities. When appointed Head of the Department of Chemical Technology (1972) he thoroughly modernized chemical technology curricula offered to students.

Selected publications

1. Bortel E., Synthetic water-soluble polymers, in: Handbook of Plastics, Olabisi O. (Ed.), Marcel-Dekker Inc. NY, 1997, pp. 291–329.
2. Bortel E., Lamot R., Untersuchung des Abbaus hochmolekularer Polyathylenoxide im Festzustand, Makromol. Chem., 178: 2617–2628, 1977.
3. Bortel E., Hodorowicz S., Lamot R., Relation between crystallinity degree and stability in solid state of high molecular poly(ethylene oxide)s, Makromol. Chem., 180, 2491–2498, 1979.
4. Bortel E., Kochanowski A., Molecular properties of high molecular weight poly(ethylene oxide)s in aqueous solutions. Determination of molecular weights and related parameters, Makromol. Chem. Rapid Commun., 1, 205–210, 1980.
5. Bortel E., Stysło M., On the structure of radically obtained maleic anhydride/C_4-alkene copolymers, Makromol. Chem., 189, 1155–1165, 1988.
6. Bortel E., Stysło M., On the chemical modifications of maleic anhydride/isobutene copolymer by means of hydrolysis, ammoniation or aminations, Makromol. Chem., 191, 2653–2662, 1990.
7. Bortel E., Kochanowski A., Witek E., Role of solvent in the heterophase copolymerization of maleic acid anhydride with vinyl isobutyl ether, J. Macromol. Sci. A, 32, 73–81, 1995.
8. Bortel E., Kochanowski A., Witek E., Water-soluble polymers with styrenosulfonate and maleic acid units in the backbone, Makromol. Chem. A, 195, 2611–2621, 1994.
9. Witek E., Pazdro M., Bortel E., Mechanism for base hydrolysis of poly(N-vinylformamide), J. Macromol. Sci. A, 44, 503–507, 2007.

Krystyna Dyrek

Professor of Chemistry, Honorary Professor of the Jagiellonian University, Dr habil, PhD

Research profile

Physicochemistry of solid state; Transition metal ions as catalytically active centers; Quantitative EPR spectroscopy; Radicals in starch

Vice-Rector of the Jagiellonian University (1990–93); Vice-Dean of the Faculty of Chemistry (1984–90); Head of the Inorganic Chemistry Department (1978–81, 1993–97); Vice-President of sections of the Polish Chemical Society: Solid State Chemistry (1979–84), Catalysis (1986–89) and Inorganic Chemistry (1989–92); Visiting Professor at Université P. et M. Curie, Paris, France, University of Detroit-Mercy, USA, Universities of Bologna and Torino, Italy, Universities of Jena and Leipzig, Germany, Kernforschungsanlage, Jülich, Germany, Zielinsky Institute of the Russian Academy of Sciences, Moscow.

Research topics: (i) Structure and reactivity of heterogeneous catalysts containing transition metal ions dispersed in oxide, aluminosilicate and polymeric matrices, studied with X-ray, electron diffraction, HR TEM/SEM and spectroscopic methods (EPR, IR, UV-vis, ESCA); (ii) Catalytic test reactions of hydrocarbon conversion on redox and acid-basic centers; (iii) Elaboration of standards for quantitative EPR measurements; (iv) X- and Q-band EPR studies of radical processes in native and chemically or physically modified starch.

Selected publications

1. Dyrek K., Sojka Z., Coordination and dispersion of Co^{2+} ions in CoO-MgO solid solutions, J. Chem. Soc. Farad. T. 1, 78, 3177–3185, 1982.
2. Dyrek K., Łabanowska M., ESR investigation of oxygen interaction with V_2O_5-MoO_3 catalysts, J. Catal., 81, 46–60, 1983.
3. Schlick S., Bortel E., Dyrek K., Catalysis on polymer supports, Acta Polym., 47, 1–15, 1996.
4. Dyrek K., Che M., EPR as a tool to investigate the transition metal chemistry on oxide surfaces, Chem. Rev., 97, 305–331, 1997.
5. Dyrek K., Che M., Electron spin resonance: Strength and weakness, in: Spectroscopy of Transition Metal Ions on Surfaces, Weckhuysen B.M., Van Der Voort P., Catana G. (Eds), Leuven University Press, 2000, pp. 45–67.
6. Dyrek K., Bidzińska E., Adamski A., Quantitative EPR – a versatile tool in fundamental and applied studies, Mol. Phys. Reports, 37, 9–23, 2003.
7. Dyrek K., Bidzińska E., Łabanowska M., Fortuna T., Przetaczek I., Pietrzyk S., EPR study of radicals generated in starch by microwaves or by conventional heating, Starch/Stärke, 59, 318–325, 2007.
8. Dyrek K., Bidzińska E., EPR spectroscopy as a tool for investigation of the starch structure and properties, in: Starch. Recent Progress in Biopolymer and Enzyme Technology, Tomasik P., Bertoft E., Blennow A. (Eds), Polish Soc. Food Technol., Kraków 2008, pp. 27–40.
9. Dyrek K., Coordination chemistry in heterogeneous catalysis, in: Coordination Chemistry in Poland, Ziółkowski J. (Ed.), Polish Chem. Soc., Wrocław 2008, pp. 395–413.

Maria Paluch

Professor of Chemistry, Dr habil, PhD

Research profile

Physical chemistry of surfaces: Free surface of water; Surface potential; Surface tension; Adsorbed and Langmuir monolayers; Bio-membranes

My research associates are: Barbara Gzyl-Malcher, PhD; Beata Korchowiec, PhD; Paweł Wydro, PhD; Katarzyna Makyła, MSc, (PhD student); Katarzyna Więcław, MSc (PhD student). Currently the research interests of our group are focused on the following areas: (i) properties of adsorption monolayers at the water/air interface, and (ii) properties of insoluble monolayers spread on aqueous subphases. In the first area we have carried out investigation of the composition and interactions in mixed adsorption films, thermodynamic and electrical properties of molecules at the free surface of water. The second area covers topics related to various aspects of insoluble monolayers spread on the aqueous subphase, particularly those leading to the use of Langmuir monolayers as a model of biomembranes. The properties of Langmuir films of lipids mixed with biomolecules, such as sterols, phytohormones and drugs are investigated. My earlier research had been focused on electrical properties of the monolayers adsorbed at the water/air interface, also on application of the interfacial cell to potentiometric titration in non-conducting solvents and on stability of suspensions in aqueous and non-aqueous media.

Selected publications

1. Paluch M., Electrical properties of free surface of water and aqueous solutions, J. Colloid Interf. Sci., 84, 27–45, 2000.
2. Wydro P., Paluch M., Surface properties of cationic-nonionic mixed surfactants system, J. Colloid Interf. Sci., 245, 75–79, 2004.
3. Wydro P., Paluch M., A study of interaction of dodecylsulfobetaine with cationic and anionic surfactant in mixed micelles and monolayers at the air/water interface, J. Colloid Interf. Sci., 286, 387–391, 2005.
4. Korchowiec B., Paluch M., Corvis Y., Rogalska E., A Langmuir film approach to elucidating interactions in lipid membranes 1,2-dipalmitoyl-sn-glicero-3-phosphoethanolamine/cholesterol/metal cation systems, Chem. Phys. Lipids, 144, 127–136, 2006.
5. Wydro P., Hąc-Wydro K., Thermodynamic description of interaction between lipids in ternary Langmuir monolayers: the study of cholesterol description in membranes, J. Phys. Chem. B, 111, 2495–2502, 2007.
6. Gzyl-Malcher B., Paluch M., Studies of the lipid interactions in mixed Langmuir monolayers, Thin Solid Films, 516, 8865–8872, 2008.
7. Gzyl-Malcher B., Filek M., Makyła K., Paluch M., Differences in surface behaviour of galactolipids originating from different kind of wheat tissue cultivated in vitro, Chem. Phys. Lipids, 155, 24–30, 2008.

Zofia Stasicka

Professor of Chemistry, Dr habil, PhD

Research profile

Chemistry and photochemistry of coordination compounds and environment

Education and Professional Career: MSc, 1955, Jagiellonian University; PhD, 1964; Habilitation 1974; Assistant Professor, 1979; Associate Professor, 1987; Full Professor of Inorganic Chemistry 1995; Vice-director of the Institute of Chemistry at the Jagiellonian University, 1978–1981; Vice-Dean, 1981, and Dean of the Faculty of Chemistry of the Jagiellonian University, 1982–1987; Head of the Department of Inorganic Chemistry, 1987–1992; Head of the Chemical Education Department, 1987–2004; President of the Chemical Terminology Commission of the Polish Chemical Society, 2001–2006; President of Supervisory Board of the PROCHEMIA Foundation, 1996–present; Emeritus Professor, since 2004.

Main research interest: The research is focused on thermal or photochemical reactivity of coordination compounds. The main subjects are complexes of the first transition metal series with π-acceptors ligands, which can be used to model the systems of environmental and biochemical importance.

Publications: About 150 original papers, more than 10 review articles, 8 books or handbooks (author or co-author), 3 books (editor).

Selected publications

1. Stochel G., Stasicka Z., Brindell M., Macyk M., Szaciłowski K., Bioinorganic Photochemistry, 398 pages, Wiley, 2009.
2. Stasicka Z., Fotochemia związków koordynacyjnych w środowisku, in: Chemia Koordynacyjna w Polsce, Part I, Polish Chem. Soc., Wrocław 2008, pp. 365–380.
3. Cieśla P., Mytych P., Kocot P, Stasicka Z., Role of iron and chromium complexes in environmental self-cleaning processes, Sep. Sci. Technol., 42, 1651–1666, 2007.
4. Jaworska M., Stasicka Z., Structure and UV-vis spectroscopy of Roussin black salt $[Fe_4S_3(NO)_7]^-$, J. Mol. Struct., 785, 68–75, 2006.
5. Chmura A., Szaciłowski K., Stasicka Z., The role of photoinduced electron transfer processes in photodegradation of the $[Fe_4(\mu_3\text{-}S)_3(NO)_7]^-$ cluster, Nitric Oxide, 15, 370–379, 2006.
6. Stasicka Z., Achmatowicz O., Kompendium terminologii chemicznej, zalecenia IUPAC, 623 pages., ZamKor, Kraków 2005.

The PRO CHEMIA Foundation

The PRO CHEMIA Foundation was established at the Faculty of Chemistry in 1995. Its main goal is to support the Faculty and to promote it in Poland and abroad.

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Contact Information:
Mailing address: PRO CHEMIA Foundation, Faculty of Chemistry, Jagiellonian University, 30-060 Kraków, Ingardena 3, Poland
Telephone: +48-12-6632206, +48-12-6632911, Fax: +48-12-663 22 06,
E-mail: prochem@chemia.uj.edu.pl,
Website: http://www.chemia.uj.edu.pl/prochemia.html