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Senior Academic Staff

Małgorzata Barańska

Professor of Chemistry, Dr habil, PhD

Research profile

Molecular spectroscopy; Raman and IR spectroscopy; Mapping and imaging; Quantum-chemical calculation; Bioactive compounds; Drugs; Metabolites

I am associated with the Faculty of Chemistry of the Jagiellonian University since my chemistry studies. From this Faculty I received my academic degrees: MSc in 1992 (*Studies of methane oxidation on the Pd/SiO2 catalyst*), PhD in 1999 (*Studies of molecular structures of cimetidine and famotidine and their complexes with metal ions by means of spectroscopic techniques*), and habilitation in 2007 (*Application of Raman mapping to in situ analysis of bioactive compounds*). Since 2009 I am head of *Raman Imaging Group*.

I am a member of Editorial Boards of the following journals: *Spectroscopy: An International Journal, E-journal of Chemistry, Biomedical Spectroscopy & Imaging (IOS)* and *Pure and Applied Chemical Sciences (Hikari Ltd)*. Appointed to Scientific Committees, I have been engaged in organising several conferences, such as 16th International Carotenoid Symposium (2011), XII International Conference on Molecular Spectroscopy (2013), Seminar on Vibrational Biospectroscopy and Imaging (2013, 2012, 2010, 2009), and International Conference SPEC 2014 (as a chairperson).

In my work I focus on research of bioactive compounds by means of spectroscopic methods, particularly modern Raman techniques. The scientific projects that I carry out are concerned with the analysis of secondary metabolites of plants that may be applied as drugs, pigments or spices. I am also interested in studying pigments and natural dyes used in art conservation. The very new direction of my research is related to lifestyle diseases, their development and methods of curing, specifically to finding new drugs with endothelium bioactivity. This research is conducted partly in a newly established Jagiellonian Centre for Experimental Therapeutics (JCET), of which I am a member.

Selected publications

1. Majzner K., Kaczor A, Kachamakova-Trojanowska N., Fedorowicz A., Chłopicki S., Barańska M., 3D Raman imaging of endothelial cells and vascular wall: perspectives in analytical spectroscopy of biomedical research, Analyst, 138, 603–610, 2013.
2. Wróbel T.P., Marzec K., Majzner K., Kochan K., Bartus M., Chlopicki S., Barańska M., Attenuated Total Reflection Fourier Transform Infrared (ATR-FTIR) spectroscopy of a single endothelial cell, Analyst, 137, 4135–4139, 2012.
3. Barańska M., Kaczor A., Morphine studied by vibrational spectroscopy and DFT calculations, J. Raman Spectr., 43, 102–107, 2012.
4. Kaczor A., Barańska M., Insight into carotenoid structure in a single microalgae cell: in situ Raman measurement of astaxanthin in *Haematococcus Pluvialis* under thermal stress conditions, Anal. Chem., 83, 7763–7770, 2011.

Marek Boczar

Dr habil, PhD

Research profile

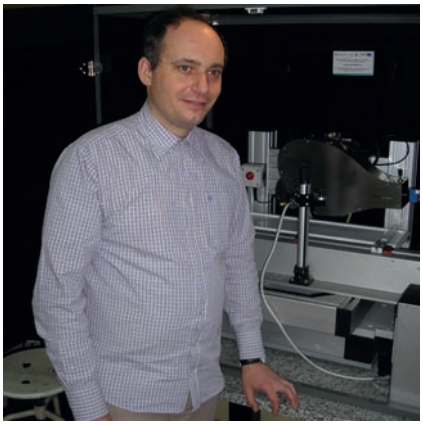
Major fields: Molecular spectroscopy; Theory of the infrared spectra; Hydrogen bonds; Fine structure of X-H bands in hydrogen bonded systems; Adiabatic approximation in vibrational calculations; Resonance interaction; Fermi resonance; Isotopic effects; Shapes and widths of infrared bands; Vibrational 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.

Marcin Broniatowski

Dr habil, PhD



Research profile

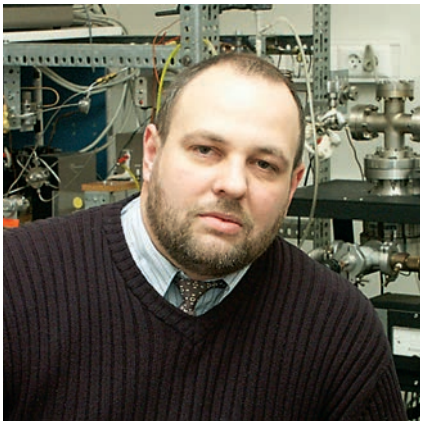
Langmuir monolayers; Physical chemistry of lipids; Fluorinated surfactants; Modeling of biomembranes; Surface activity of terpenes

Academic career: 2000 – MA thesis regarding crystallography of macrocyclic organic compounds, 2004 – PhD thesis regarding the surface activity of semifluorinated alkanes, 2011 – habilitation summarizing the publications regarding fluorinated surfactants, 2004 till now – I am employed at the Faculty of Chemistry of the Jagiellonian University.

My scientific activity concerns the application of Langmuir monolayers as a versatile platform for the physicochemical characterization of surfactants as well as for biomembranes' modeling. By now in my studies I focused on the following topics: physicochemical characterization of Langmuir monolayers formed by different fluorinated surfactants, interactions of fluorinated and hydrogenated surfactants, incorporation of ion channel peptides into the model membrane, nucleation in monolayers, interaction of mercury salts with model membranes, intermolecular interactions in model lipid rafts. Recently I have been working on a project regarding the interactions of pharmaceutically active pentacyclic triterpenes with phospholipids of cellular and inner mitochondrial membranes. In my studies I apply the Langmuir technique combined with dedicated microscopies and electrochemical methods. I am especially interested in the application of synchrotron X-ray radiation in the investigation of soft matter. In my studies I apply the method of Grazing Incidence X-ray Diffraction for the characterization of thin organic films at liquid/gas interfaces and on solid supports.

Selected publications

1. Broniatowski M., Flasiński M., Wydro P., Lupane-type pentacyclic triterpenes in Langmuir monolayers: A synchrotron radiation scattering study, Langmuir, 28, 5201–5210, 2012.
2. Broniatowski M., Flasiński M., Wydro P., Broniatowska E., Self-organization of non-amphiphilic molecules. Studies of thin films of long-chain homologous dialkylthioethers at the water/air interface, J. Colloid Interface Sci., DOI: 10.1016/j.jcis.2012.12.055, 2013.
3. Broniatowski M., Flasiński M., Dynarowicz-Łątka P., Majewski J., Grazing incidence diffraction and X-ray reflectivity studies of the interactions of inorganic mercury salts with membrane lipids in Langmuir monolayers at the air/water interface, J. Phys. Chem. B, 114, 9474–9484, 2010.
4. Broniatowski M., Dynarowicz-Łątka P., Semifluorinated alkanes – primitive surfactants of fascinating properties, Adv. Colloid Interface Sci., 138, 63–83, 2008.



Lucjan Chmielarz

Dr habil, PhD

Research profile

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

Prof. JU, 2011, Jagiellonian University; Habilitation, 2007, Jagiellonian University; PhD, 1997, Jagiellonian University; MSc, 1992, Jagiellonian University; Vice Dean for Students Affairs (since 2012); Head of the course of studies in Environmental Protection at the Jagiellonian University (2008–2012); 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; Elimination of organic and inorganic pollutants from wastewater; Synthesis and functionalization of catalytic systems based on cationic layered clays (e.g. PILCs, PCHs), anionic clays (LDHs), mesoporous silica and zeolites.

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; Université Pierre et Marie Curie, Paris, France; Universidad Politecnica de Valencia, Spain; University of Warwick, UK; Institute of Chemical Technology, Prague, Czech Republic.

Selected publications

1. Chmielarz L., Kuśtrowski P., Dziembaj R., Cool P., Vansant E.F., SBA-15 mesoporous silica modified with metal oxides by MDD method in the role of DeNOx catalysts, Micropor. Mesopor. Mat., 127, 133–141, 2010.
2. Chmielarz L., Piwowarska Z., Kuśtrowski P., Węgrzyn A., Gil B., Kowalczyk A., Dudek B., Dziembaj R., Michalik M., Comparison study of titania pillared interlayered clays and porous clay heterostructures modified with copper and iron as catalysts of the DeNOx process, Appl. Clay Sci., 53, 164–173, 2011.
3. Chmielarz L., Wojciechowska M., Rutkowska M., Adamski A., Węgrzyn A., Kowalczyk A., Dudek B., Boroń P., Michalik M., Matusiewicz A., Acid-activated vermiculites as catalysts of the DeNOx process, Catal. Today, 191, 25–31, 2012.
4. Chmielarz L., Jabłońska M., Strumiński A., Piwowarska Z., Węgrzyn A., Witkowski S., Michalik M., Selective catalytic oxidation of ammonia to nitrogen over Mg-Al, Cu-Mg-Al and Fe-Mg-Al mixed metal oxides doped with noble metals, Appl. Catal. B, 130–131, 152–162, 2013.

Dariusz Cież

Dr habil, PhD

Research profile

Metalorganics; Chiral catalysts; Transition metal complexes; Organic redox processes

My field of interest is related to organic synthesis promoted by both metalorganics and transition metal complexes. My current investigations are focused on titanium(IV)-mediated aldol-like reactions, such as Mannich and nitro-Mannich processes, oxidative coupling of 2-substituted carboxylates, and Ce(IV) mediated redox heterocyclizations. The research is conducted within the *Biologically-Active Heterocyclic Compounds* team that is a subunit of *Organic Physicochemistry* Group, and for whose work I am responsible. More information on our research is available at http://www.chemia.uj.edu.pl/~trzewik/Strona1eng.html.

Selected publications

1. Michalski O., Cież D., Chiral isothiocyanates – an approach to determination of the absolute configuration using circular dichroism measurement, J. Mol. Struct., 1037, 225–235, 2013.
2. Cież D., Kalinowska-Tłuścik J., Marchewka J., An approach to 2,3-diaminosuccinic acid derivatives – synthesis of 2-thioxo-1,3-imidazolidines via Mannich reaction, Aust. J. Chem., 65, 333–342, 2012.
3. Cież D., Kalinowska-Tłuścik J., Titanium(IV) enolates of 2-nitrocarboxylic esters and their oxidative chlorination. A convenient route to α-chloro-α-nitrocarboxylates, Synlett, 23, 267–271, 2012.
4. Cież D., Kalinowska-Tłuścik J., Enolates of 2-isothiocyanatocarboxylic esters – Synthesis of thiazolo[5,4-d] thiazole derivatives and 2-thioxo-1,3-thiazolidine-4-carboxylates, Synthesis, 44, 1736–1744, 2012.
5. Cież D., Svetlik J., A one-pot preparation of 5-oxo-2,4-disubstituted-2,5-dihydro-1H-imidazol-2-carboxylates from α-bromoesters, Synlett, 3, 315–318, 2011.
6. Cież D., A direct preparation of N-unsubstituted pyrrole-2,5-dicarboxylates from 2-azidocarboxylic esters, Org. Lett., 11, 4282–4285, 2009.
7. Trzewik B., Cież D., Hodorowicz M., Stadnicka K., New-α-amido-α-aminonitrones as building-blocks for constructing heterocyclic systems, Synthesis, 40, 2977–2985, 2008.
8. Cież D., Kalinowska-Tłuścik J., Peyrat S., Pougoue Touko E., Trzewik B., Zwoliński K., A simple synthesis of new 2-thioxoimidazolidine-4,5-dicarboxylates from vicinal diisothiocyanatocarboxylates, Synthesis, 40, 3261–3266, 2008.
9. Cież D., Titanium(IV)-mediated synthesis of 2,3-diisothiocyanato-succinic acid diesters and 3,6-dithioxo-piperazine derivatives, Tetrahedron, 63, 4510–4515, 2007.

Patrycja Dynarowicz-Łątka

Professor of Chemistry, Dr habil, PhD

Research profile

Physical chemistry of interfaces; Surface chemistry

I am Head of the Physicochemistry of Interfacial Phenomena Group. In my research I focus on the properties of interfaces (gas, liquid and solid). Specific areas of interest are:

1. Highly ordered organic thin films. Using Langmuir-Blodgett (LB) deposition or self-assembly, films can be formed as thin as a single molecular layer with very good control over structure. Especially with the LB method, highly ordered, defect-free ultrathin films with controllable molecular orientation, thickness and architecture can be made for optical devices, highly specific chemical sensors and molecular electronics.

2. Molecular interactions in monolayers. In this area of research cellular membranes are modeled with the Langmuir monolayer technique and the interaction between membrane components and various biomolecules, mainly drugs, are investigated. The aim of this work is to understand the mode of action of these drugs on membrane level.

3. Synthesis and physico-chemical characterization of surface active molecules. In this project, the synthesis of novel surfactants of classical amphiphilic structure as well as of non-typical surface active molecules is performed. For their characterization, various optical and spectroscopical methods are used.

Selected publications

1. Hąc-Wydro K., Lenartowicz R., Dynarowicz-Łątka P., The influence of plant stanol (β-sitostanol) on inner leaflet of human erythrocytes membrane modeled with the Langmuir technique, Colloids Surf. B, 102, 178–188, 2013.
2. Mildner J., Dynarowicz-Łątka P., β-carotene does not form a true Langmuir monolayer at the air/water interface, Colloids Surf. B, 90, 244–247, 2012.
3. Hąc-Wydro K., Zając A., Dynarowicz-Łątka, P., The influence of plant stanol on phospholipid monolayers – the effect of phospholipid structure, J. Colloid Interface Sci., 360, 681–689, 2011.
4. Hąc-Wydro K., Dynarowicz-Łątka, P., Effect of edelfosine on tumor and normal cells model membranes – a comparative study, Colloids Surf. B, 76, 366–369, 2010.
5. Dynarowicz-Łątka P., Milart P., Synthesis and Langmuir monolayer characterization of the nitro derivatives of polyphenyl carboxylic acids, J. Chem. Res., 4, 225–228, 2009.
6. Miñones Jr. J., Pais S., Miñones J., Conde O., Dynarowicz-Łątka P., Interactions between membrane sterols and phospholipids in model mammalian and fungi cellular membranes – a Langmuir monolayer study, Biophys. Chem., 140, 69–77, 2009.
7. Osak A., Dynarowicz-Łątka P., Conde O., Miñones Jr J., Pais S., Edelfosine – a new antineoplastic drug based on a phospholipid-like structure. The Langmuir monolayer study, Colloids Surf. A, 319, 71–76, 2008.
8. Hąc-Wydro K., Dynarowicz-Łątka P., Grzybowska J., Borowski E., Interactions between amphotericin B 3-(N',N'-dimethylamino) propyl amide and cellular membrane components in Langmuir monolayers, Thin Solid Films, 516, 1197–1203, 2008.

Andrzej Eilmes

Dr habil, PhD

Research profile

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

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 or ionic liquids, and on solvent effects on ion complexation and absorption spectra. 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. 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.
8. Eilmes A., Kubisiak P., Molecular Dynamics study on the effect of Lewis acid centers in poly(ethylene oxide)/$LiClO_4$ polymer electrolyte, J. Phys. Chem. B, 115, 14938–14946, 2011.
9. Eilmes A., TDDFT study of absorption spectrum of ketocyanine dye complexes with metal ions: explicit solvent model, Theor. Chem. Acc., 127, 743–750, 2010.
10. Eilmes A., Ab initio Molecular Dynamics simulations of ketocyanine dyes in organic solvents, in: Bubak M., Szepieniec T., Wiatr K. (Eds.) PL-Grid 2011, Lecture Notes in Computer Science 7136, Springer-Verlag 2012, pp. 276–284.

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); Bologna Expert; Member of EURASHE Council.

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 acetyl-cholinesterase 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 pronciple, 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.
10. Frankowicz M., Bugaj J., Kozielska A., Navigating complexity: management of change in Polish higher education, Manage. Technol. Changes, 1, 293–296, 2009.

Barbara Gil

Dr habil, PhD

Research profile

Zeolites; Metal-Organic-Frameworks (MOFs); Synthesis; Characterization; Drug delivery; IR spectroscopy

Since my graduation I have been working in the fascinating area of crystalline porous materials: zeolites, zeotypes, mesoporous materials. They are extensively used in various practical application and constantly yield new discoveries. Recently, I started investigating two new classes of these materials: so-called two-dimensional zeolites producing ultrathin crystals and metal-organic-frameworks with tuneable channel dimensions and unlimited diversity. Additional focus of my research is the possible use of MOFs and zeolites as carriers for biologically active compounds in drug delivery and targeted therapies.

My investigation of the state of the art materials is possible thanks to many collaborations with excellent scientists. I am cooperating, among others, with the Czech and Polish Academy of Sciences, Faculty of Pharmacy of the Jagiellonian University, University of St. Andrews, Scotland, Christian Albrecht Universität, Kiel, Germany, Caen University, France.

For my research I have been awarded by UJ Rector's Award for outstanding scientific achievements (1993, 1998, 2001, 2003, 2008, 2009), gained scholarship of the Foundation for Polish Science (1996), and the award from the Ministry of National Education (2000, 2005).

Selected publications

1. Serrano D. P., Garcia R. A., Linares M., Gil B., Influence of the calcination treatment on the catalytic properties of hierarchical ZSM-5, Catal. Today, 179, 91–101, 2012.
2. Reimer N., Gil B., Marszalek B., Stock N., Thermal post-synthetic modification of AlMIL-53-COOH: systematic investigation of the decarboxylation and condensation reaction, CrystEngComm, 41, 4036–4044, 2012.
3. Pérez-Mayoral E., Musilová Z., Gil B., Marszalek B., Položij M., Nachtigall P., Čejka J., Synthesis of quinolines via Friedländer reaction catalyzed by CuBTC Metal-Organic-Framework, Dalton Trans., 41, 4036–4044, 2012.
4. Reinsch H., Marszałek B., Wack J., Senker J., Gil B., Stock N., A new Al-MOF based on a unique column-shaped inorganic building unit exhibiting strongly hydrophilic sorption behavior, Chem. Commun., 48, 9486–9488, 2012.
5. Micek-Ilnicka A., Gil B., Heteropolyacid encapsulation into the MOF: influence of acid particles distribution on ethanol conversion in hybrid nanomaterials, Dalton Trans., 41, 12624–1262, 2012.
6. Reinsch H., Van der Veen M., Gil B., Marszalek B., de Vos D., Stock N., Structures, sorption characteristics and nonlinear optical properties of a new series of highly stable aluminium MOFs, Chem. Mater., 25, 17–26, 2013.

Kinga Góra-Marek

Dr habil, PhD

Research profile

Micro- and mesoporous materials; Zeolites; IR spectroscopy; Catalysis

Kinga Góra-Marek completed her PhD at the Jagiellonian University (2001–2005) under the supervision of Professor Jerzy Datka. The thesis was on the characterization of zeolite catalysts, their acid properties in particular. Between 2005 and 2006 she worked as a postdoc in the Institute of Chemical Technology (ITQ) in Valencia under the supervision of Professor Avelino Corma and Dr. Patricia Concepción Heydorn.

The main research activity of Dr. Kinga Góra-Marek is focused on the characterization of solid catalysts, e.g. the nature of their active sites, the activation of molecules participating in catalytic reactions, and mechanisms of reactions catalyzed by heterogeneous catalysts (zeolites, micro- and mesoporous materials). The main spectroscopic tool used in this research is IR supported by other techniques, such as NMR, EPR, XRD, adsorption studies, and catalytic tests.

Current cooperation: Institute of Catalysis and Surface Chemistry of the Polish Academy of Sciences, Institute of Nuclear Physics of the Polish Academy of Sciences, Institute of Chemical Technology (ITQ) in Valencia, University of Antwerp.

Selected publications

1. Góra-Marek K., Vib. Spectrosc., 58, 104–108, 2012.
2. Pietrzyk P., Dujardin C., Góra-Marek K., Granger P., Sojka Z., Phys. Chem. Chem. Phys., 14, 2203–2215, 2012.
3. Góra-Marek K., Glanowska A., Datka J., Micropor. Mesopor. Mat., 158, 162–169, 2012.
4. Lalowicz Z.T., Stoch G., Birczyński A., Punkkinen M., Ylinen E.E., Krzystyniak M., Góra-Marek K., Datka J., Solid State Nuc. Mag. Reson., 45–46, 66–74, 2012.
5. Góra-Marek K., Palomares A.E., Glanowska A., Sadowiska K., Datka J., Micropor. Mesopor. Mat., 162, 175–180, 2012.
6. Sadowska K., Góra-Marek K., Datka J., Vib. Spectrosc., 63, 418–425, 2012.
7. Sadowska K., Góra-Marek K., Drozdek M., Kuśtrowski P., Datka J., Martinez Triguero J., Rey F., Micropor. Mesopor. Mat.,168, 195–205, 2013.

Tad A. Holak

Professor of Chemical Biology, PhD

Research profile

Chemical biology; Biochemistry; Tumor; NMR

Head of a research group: Translational Chemical Biology and Drug Discovery, starting 2012.

The research interests of the group lie in the emerging area of chemical biology. We study biologic processes underlying growth and proliferation of human cancer cells using small molecules as probes. Specifically, our research has uncovered many remarkable small-molecule probes of protein-protein interactions that are at the root of human cancer. New drugs have been developed whose therapeutic effects are the direct consequence of proteins and/or cellular mechanisms revealed by our group research (for example, small molecules of oncogenic proteins, Mdm2 and Mdmx, which inhibit the tumor suppressor p53 protein. p53 – "the guardian of the genome" – has an overarching role in protecting the organism from cancer).

Selected publications

1. Schnuchel A., Wiltscheck R., Czisch M., Herrler M., Willimsky G., Graumann P., Marahiel M.A., Holak T.A., Structure in solution of the major cold shock protein from *Bacillus Subtilis*, Nature, 364, 169–171, 1993.
2. Fucini P., Renner C., Heberhold C., Mühlhahn P., Noegel A.A., Holak, T.A., The repeating segments of the F-actin cross-linking gelation factor have an immunoglobulin-like fold, Nature Struct. Biol., 4, 223–230, 1997.
3. Krajewski M., Ozdowy P., D'Silva L., Rothweiler U., Holak T.A., NMR indicates that the small molecule RITA does not block the p53-MDM2 binding in vitro, Nature Medicine 11, 1135–1136, 2005.
4. Riedl J., Crevenna A.H., Kessenbrock K., Yu J.H., Neukirchen D., Bista M., Bradke F., Jenne D., Holak T.A., Werb Z., Sixt M., Wedlich-Soldner R., Lifeact: a versatile marker to visualize F-actin, Nature Methods, 5, 605–607, 2008.
5. Bista M., Kowalska K., Janczyk W., Dömling A., Holak T.A., Robust NMR screening for lead compounds using tryptophan-containing proteins, J. Am.. Chem. Soc., 131, 7500–7501, 2009.
6. Sitar T., Gallinger J., Ducka A.M., Ikonen T.P., Wohlhoefler M., Schmoller K.M., Bausch A.R., Joel P., Trybus K.M., Noegel A.A., Schleicher M., Huber R., Holak T.A., Molecular architecture of the Spire-actin nucleus and its implication for actin filament assembly, Proc. Nat. Acad. Sci. USA, 108, 19575–19580, 2011.
7. Popowicz G.M., Doemling A., Holak T.A., The structure-based design of Mdm2/Mdmx-p53 inhibitors gets serious, Angew. Chem. Int. Ed., 50, 2680–2688, 2011.
8. Mishra S.K., Ammon T., Popowicz G.M., Krajewski M., Nagel R.J., Ares M. Jr., Holak T.A., Jentsch, S., Role of the ubiquitin-like protein Hub1 in splice site usage and alternative splicing, Nature, 474, 173–178, 2011.
9. Baek S., Kutchukian P.S., Verdine G.L, Huber R., Holak T.A., Structure of the stapled p53 peptide bound to Mdm2, J. Am. Chem. Soc., 134, 103–106, 2012.

Marian Jaskuła

Professor of Chemistry, Dr habil, PhD

Research profile

Physical chemistry; Electrochemistry; Metal deposition and dissolution; Industrial electrolysis; Materials science; Nanotechnology; New nanostructured materials; Lithium ion batteries

Born 1948; Education: MSc 1971, PhD 1978, Habilitation 1992 (Rheinisch Westfälische Technische Hochschule Achen Germany); Research fellow of Alexander von Humboldt Foundation 1987; Head the *Electrochemistry* group at the Jagiellonian University since 1992; Ausserplanmässiger Professor RWTH Aachen (Germany) 1999; Honorary Professor at Kiev National University of Technology & Design (Ukraine); General Secretary of scientific society Societas Humboldtiana Polonorum since 2004.

International cooperation: Technical University IME Aachen (Germany), University of Hamburg (Germany), Danmarks Tekniske Universiteit Lyngby (Denmark), Kiev National University of Technology & Design Ukraine, Penza State University Russia.

The interest of the *Electrochemistry* group concentrates on various aspects of basic and industrial electrochemistry, especially on the field of non-ferrous and noble metals (copper electrorefining process at high current densities, mechanism and kinetics of silver ion cementation on metallic copper, deposition and dissolution of metals and alloys, and corrosion), and on new materials and nanotechnology (nanoporous and self organizing structures of aluminum and titanium oxides obtained by anodization synthesis of metallic nanowires, such as Ag, Au, Cu, Sn. Sb, using porous alumina matrix, new nanostructural electrode materials for lithium-ion batteries, and metallic nanowires for electrochemical sensors).

More information on the activity of the group: http://www.chemia.uj.edu.pl/zchfze/

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. 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.
3. Tang P.T., Jaskuła M., Kubiczek M., Mizushima I., Pantleon K., Arentoft M., Pulse reversal plating of nickel-cobalt alloys, Trans. Inst. Met. Finish., 87, 72–77, 2009.
4. Zaraska L., Kurowska E., Sulka G.D., Jaskuła M., Porous alumina membranes with branched nanopores as templates for fabrication of Y-shaped nanowire arrays, J. Solid State Electrochem., 16, 3611–3619, 2012.

Mariusz Kępczyński

Dr habil, PhD

Research profile

Dispersed systems for biomedical applications; Vesicular structures

My research falls within the area of colloid and surface chemistry, polymers, and photochemistry, and focuses on structure and dynamics of lipid/surfactant systems and photosensitizers for photodynamic therapy. Research topics are inspired by medical and pharmaceutical problems and include:

- porphyrins with covalently attached polymer chains as sensitizers in PDT
- lipid and surfactant vesicles as drug vehicles
- nanocapsules and nanoparticles made from silica and silicone materials
- liposomes as a model of biological membranes.

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Selected publications

1. Stępniewski M., Kepczynski M., Jamróz D., Nowakowska M., Rissanen S., Vattulainen I., Róg T., Interaction of hematoporphyrin with lipid membranes, J. Phys. Chem. B, 116, 4889–4897, 2012.
2. Kepczynski M., Jamróz D., Wytrwal M., Bednar J., Rzad E., Nowakowska M., Interactions of a hydrophobically modified polycation with zwitterionic lipid membranes, Langmuir, 28, 676–688, 2012.
3. Kepczynski M., Kumorek M., Stępniewski M., Róg T., Kozik B., Jamróz D., Bednar J., Nowakowska M., Behavior of 2,6-bis-decyloxynaphthalene inside lipid bilayer, J. Phys. Chem. B, 114, 15483–15494, 2010.
4. Jamróz D., Kepczynski M., Nowakowska M., Molecular structure of the dioctadecyldimethylammonium bromide (DODAB) bilayer, Langmuir, 26, 15076–15079, 2010.
5. Kepczyński M., Bednar J., Kuźmicz D., Wydro P., Nowakowska M., Spontaneous formation of densely stacked multilamellar vesicles in dioctadecyldimethylammonium bromide/oleosiloxane mixtures, Langmuir, 26, 1551–1556, 2010.
6. Nawalany K., Kozik B., Kępczyński M., Zapotoczny S., Kumorek M., Nowakowska M., Jachimska B., Properties of polyethylene glycol supported tetraarylporphyrin in aqueous solution and its interaction with liposomal membranes, J. Phys. Chem. B, 112, 12231–12239, 2008.
7. Kępczyński M., Lewandowska J., Romek M., Zapotoczny S., Ganachaud F., Nowakowska M., Silicone nanocapsules templated inside the membranes of catanionic vesicles, Langmuir, 23, 7314–7320, 2007.
8. Kępczyński M., Karewicz A., Górnicki A., Nowakowska M., Interactions of porphyrin covalently attached to poly(methacrylic acid) with liposomal membranes, J. Phys. Chem. B, 109, 1289–1294, 2005.

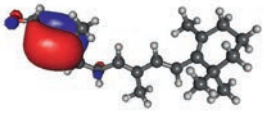
Jacek Korchowiec

Dr habil, PhD

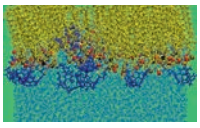
Research profile

Quantum Chemistry; Theory of Chemical Reactivity; Polarizable Force Fields; Molecular Dynamics

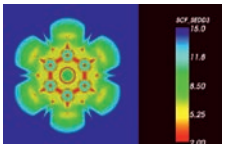
Head of K. Gumiński Department of Theoretical Chemistry; Visiting Researcher at Hannover University, National Institute of Materials and Chemical Research in Tsukuba, Hiroshima University, Kyushu University; Visiting Professor at Kyushu University and Lorraine University. My research is focused on the following topics: linear scaling methods, inclusion phenomena, conceptual density functional theory, molecular dynamics (MD) description of monolayers at water/air interfaces, bond detectors, polarizable force fields and energy partitioning schemes. Among my achievements are: charge sensitivity analysis, self-consistent charge and configuration method for subsystems, self-consistent method for subsystems, regional localized molecular orbitals (RLMO), elongation and elongation cutoff methods.



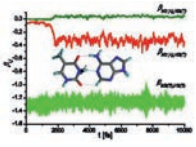
RLMO



Monolayer at water/air interface



Single exponential decay detector



Bond-detectors for MD simulations

Selected publications

1. Stachowicz A., Rogalski M., Korchowiec J., Charge sensitivity approach to mutual polarization of reactants: Molecular mechanics perspective, J. Mol. Model., DOI 10.1007/s00894-013-1757-4, 2013.
2. de Silva P., Korchowiec J., Wesolowski T., Revealing the bonding pattern from the molecular electron density using single exponential decay detector: An orbital-free alternative to the electron localization function, Chem. Phys. Chem., 13, 3462–3465, 2012.
3. de Silva P., Korchowiec J., Fast orbital localization scheme in molecular fragments resolution, Phys. Chem. Chem. Phys., 14, 546–552, 2012.
4. de Silva P., Korchowiec J., Energy partitioning scheme based on self-consistent method for subsystems: Populational space approach, J. Comput. Chem., 32, 1054–1064, 2011.
5. Korchowiec B., Korchowiec J., Hato M., Rogalska E., Glycolipid-cholesterol monolayers: Towards a better understanding of the interaction between the membrane components, Biochim. Biophys. Acta-Biomembranes, 1808, 2466–2476, 2011.

Paweł Kościelniak

Professor of Chemistry, Dr habil, PhD

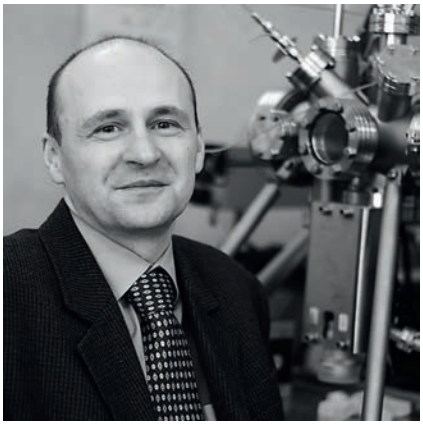
Research profile

Analytical chemistry; Flow analysis; Environmental chemistry, 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 in environmental and forensic chemistry. For instance, we are the authors of a versatile flow injection manifold allowing different calibration methods to be realized in a simple, fast and cost-effective manner. In addition, we are focused on miniaturization of flow systems and their adaptation to clinical and forensic analysis. 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 HPLC-MS, GC-MS, CE-MS, ICP-MS, ICP-OES, AAS, and AFS. Apart from the above research we offer attractive courses of studies that give students a chance to exploit analytical knowledge and skills in environmental, toxicological and forensic areas.

Selected publications

1. Kozak J., Gutowski J., Kozak M., Wieczorek M., Kościelniak P., New method for simultaneous determination of Fe(II) and Fe(III) in water using flow injection technique, Anal. Chim. Acta, 668, 8–12, 2010.
2. Zięba-Palus J., Trzcińska B., Kościelniak P., Comparative analysis of car paint traces in terms of colour by vis microspectrometry for forensic needs, Anal. Lett., 43, 436–445, 2010.
3. Wietecha-Posłuszny R., Garbacik A., Woźniakiewicz M., Kościelniak P., Microwave-assisted hydrolysis and extraction of tricyclic antidepressants from human hair, Anal. Bioanal. Chem., 399, 3233–3240, 2011.
4. Kozak J., Jodłowska N., Kozak M., Kościelniak P., Simple flow injection method for simultaneous spectrophotometric determination of Fe(II) and Fe(III), Anal. Chim. Acta, 702, 213–217, 2011.
5. Wietecha-Posłuszny R., Garbacik A., Woźniakiewicz M., Moos A., Wieczorek M., Kościelniak P., Application of microextraction by packed sorbent for isolation of psychotropic drugs from human serum, Anal. Bioanal. Chem., 402, 2249–2257, 2012.
6. Król M., Kula A., Wietecha-Posłuszny R., Woźniakiewicz M., Kościelniak P., Examination of black inkjet printing inks by capillary electrophoresis, Talanta, 96, 236–242, 2012.
7. Wietecha-Posluszny R., Woźniakiewicz M., Garbacik A., Chęsy P., Kościelniak P., Application of microwave irradiation to fast and efficient isolation of benzodiazepines from human hair, J. Chromatogr. A, 1278, 22–28, 2013.



Andrzej Kotarba

Dr habil, PhD

Research profile

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

Appointments: PhD studies Coordinator; Head of Inorganic Chemistry Department and 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. Maniak G., Stelmachowski P., Kotarba A., Sojka Z., Rico-Pérez V., Bueno-López A., Rationales for the selection of the best precursor for potassium doping of cobalt spinel based deN_2O catalyst, Appl. Catal. B, 136-137, 302–307, 2013.
2. Legutko P., Stelmachowski P., Trębala M., Sojka Z., Kotarba A., Role of electronic factor in soot oxidation process over tunnelled and layered potassium iron oxide catalysts, Top. Catal., DOI: 10.1007/s11244-013-0003-8.
3. Cieślik M., Zimowski S., Gołda M., Engvall K., Pan J., Rakowski W., Kotarba A., Engineering of bone fixation metal implants biointerface – application of Parylene C as versatile protective coating, Mater. Sci. Eng. C, 32, 2431–2435, 2012.
4. Cieślik M., Kot M., Reczyński W., Engvall K., Rakowski W., Kotarba A., Parylene coatings on stainless steel 316 L surface for medical applications – Mechanical and protective properties, Mater. Sci. Eng. C, 32, 31–35, 2012.
5. Piskorz W., Zasada F., Stelmachowski P., Diwald O., Kotarba A., Sojka Z., Computational and experimental investigations into N_2O decomposition over MgO nanocrystals – From thorough molecular mechanism to ab initio microkinetics, J. Phys. Chem. C, 115, 22451–22460, 2011.
6. Kotarba A., Bieniasz W., Kuśtrowski P., Stadnicka K., Sojka Z., Composite ferrite catalyst for ethylbenzene dehydrogenation: Enhancement of potassium stability and catalytic performance by phase selective doping, Appl. Catal. A, 407, 100–105, 2011.
7. Maniak G., Stelmachowski P., Stanek J.J., Kotarba A., Sojka Z., Catalytic properties in N_2O decomposition of mixed cobalt–iron spinels, Catal. Commun., 15, 127–131, 2011.

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, 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 native and immobilized urease, and interfacial phonemena taking place in the urease system.

Selected publications

1. Krajewska B., Wydro P., Kyzioł A., Chitosan as a subphase disturbant of membrane lipid monolayers. The effect of temperature at varying pH: I. DPPG, Colloids Surf. A, in press.
2. Krajewska B., van Eldik R., Brindell M., Temperature- and pressure-dependent stopped-flow kinetic studies of jack-bean urease. Implications for the catalytic mechanism, J. Biol. Inorg. Chem., 17, 1123–1134, 2012.
3. Krajewska B., Hydrogen peroxide-induced inactivation of urease. Mechanism, kinetics and inhibitory potency, J. Mol. Catal. B: Enzym., 68, 262–269, 2011.
4. Krajewska B., Wydro P., Jańczyk A., Probing the modes of antibacterial activity of chitosan. Effects of pH and molecular weight on chitosan interactions with membrane lipids in Langmuir films, Biomacromolecules, 12, 4144–4152, 2011.
5. Krajewska B., Ureases. I. Functional, kinetic and catalytic properties: a review, J. Mol. Catal. B: Enzym., 59, 9–21, 2009.
6. Krajewska B., Ureases. II. Properties and their customizing by enzyme immobilizations: a review, J. Mol. Catal. B: Enzym., 59, 22–40, 2009.
7. Alatorre-Meda M., Taboada P., Sabin J., Krajewska B., Varela L.M., Rodriguez J.R., DNA-chitosan complexation: A DLS study, Colloids Surf. A, 339, 145–152, 2009.
8. Krajewska B., Mono- (Ag, Hg) and di- (Cu, Hg) valent metal ions effects on the activity of jack bean urease, J. Enzym. Inhib. Med. Chem., 23, 535–542, 2008.
9. 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. Membr. Sci., 273, 124–128, 2006.
10. 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.
11. Krajewska B., Membrane-based processes performed with use of chitin/chitosan materials, Sep. Purif. Technol., 41, 305–312, 2005.

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; Ordered mesoporous carbons

Habilitation, 2007, Jagiellonian University; PhD, 2000, Jagiellonian University; MSc, 1995, Jagiellonian University; Head of research group of Organic Technology (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 different deposition techniques for functionalization of mesoporous molecular sieve surface; 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; Development of new methods for synthesis of ordered mesoporous carbons for catalytic and adsorption applications.

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. 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.
5. Janus R., Kuśtrowski P., Dudek B., Piwowarska Z., Kochanowski A., Michalik M., Cool P., Removal of methyl-ethyl ketone vapor on polyacrylonitrile-derived carbon/mesoporous silica nanocomposite adsorbents, Micropor. Mesopor. Mat., 145, 65–73, 2011.

Krzysztof Lewiński

Professor of Chemistry, Dr habil, PhD

Research profile

Crystallography; Crystal structure; Proteins; Structural biology; Biological chemistry; High-pressure crystallography

Head of the Department of Crystal Chemistry and Crystal Physics; Head of Biocrystallography research group; Founding member and treasurer of the Polish Crystallographic Association (2010–2013), member of the Crystallography Committee of the Polish Academy of Sciences (2007–2011, 2011–2014).

Research interest is focused on structural investigations of proteins and small molecules by X-ray diffraction methods. Among recent projects are: specificity and thermodynamics of ligand binding by beta-lactoglobuline; modified lactoglobulin variants with increased specificity for binding selected compounds; structural investigations of interactions between human transcription factor YY1 and DNA; determination of high-pressure crystal structure of selected proteins (ribonuclease A, insulin, BPTI, hemoglobin, thaumatin); protein-drug interactions; synthesis and structural investigations of new organic compounds with potential biological activity.

Selected publications

1. Loch J.I., Bonarek P., Polit A., Ries D., Dziedzicka-Wasylewska M., Lewiński K., Structural and thermodynamic studies of 18-carbon unsaturated fatty acids binding to bovine β-lactoglobulin, Int. J. Biol. Macromol., 57, 226–231, 2013.
2. Pinkowicz D., Kurpiewska K., Lewiński K., Bałanda M., Mihalik M., Zentkova M., Sieklucka B., High-pressure single-crystal XRD and magnetic study of a octacy-anoniobete-based magnetic sponge, CrystEngComm, 14, 5224–5229, 2012.
3. Loch J.I., Polit A., Bonarek P., Olszewska D., Kurpiewska K., Dziedzicka-Wasylewska M., Lewiński K., Structural and thermodynamic studies of binding saturated fatty acids to bovine β-lactoglobulin, Int. J. Biol. Macromol., 50, 1095–1102, 2012.
4. Mazuryk O., Kurpiewska K., Lewiński K., Stochel G., Brindell M., Interaction of apo-transferrin with anticancer ruthenium complexes NAMI-A and its reduced form, J. Inorg. Biochem., 116, 11–18, 2012.
5. Loch J.I., Polit A., Górecki A., Bonarek P., Kurpiewska K., Dziedzicka-Wasylewska M., Lewiński, K., Two modes of fatty acid binding to bovine β-lactoglobulin - crystallographic and spectroscopic studies, J. Mol. Rec., 24, 341–349, 2011.
6. Kurpiewska K., Lewiński K., High pressure macromolecular crystallography for structural biology: a review, Cent. Eur. J. Biol., 5, 531–542, 2010.
7. Kurpiewska K., Font J., Ribo M., Vilanova M., Lewiński K., X-ray crystallographic studies of RNase A variants engineered at the most destabilizing positions of the main hydrophobic core: further insight into protein stability, Protein. Struct. Funct. Bioinform., 77, 658–669, 2009.

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., Filek M., Kurdziel M., Bidzińska E., Miszalski Z., Hartikainen H., EPR spectroscopy as a tool for investigation of differences in radical status in wheat plants of various tolerances to osmotic stress induced by NaCl and PEG-treatment**,** J. Plant Physiol., 170, 136–145, 2013.
2. Łabanowska M., Wesełucha-Birczyńska A., Kurdziel M., Puch P., Thermal effects on the structure of cereal starches. EPR and Raman spectroscopy studies**,** Carbohydr. Polym., 92, 842–848, 2013.
3. Łabanowska M., Wesełucha-Birczyńska A., Kurdziel M., Sepioło K., The mechanism of thermal activated radical formation in potato starch studied by electron paramagnetic resonance and Raman spectroscopies**,** Carbohydr. Polym., 9, 339–347, 2013.
4. Łabanowska M., Filek M., Kurdziel M., Bednarska E., Dłubacz A., Hartikainen H., Electron paramagnetic resonance (EPR) spectroscopy characterization of wheat grains from plants of different water stress tolerance**,** J. Plant Physiol., 169, 1234–1242, 2012.
5. Łabanowska M., Bidzińska E., Para A., Kurdziel M., EPR investigation of Cu(II)-complexes with nitrogen derivatives of dialdehyde starch, Carbohydr. Polym., 87, 2605–2613, 2012.
6. Łabanowska M., Filek M., Kościelniak J., Kurdziel M., Kuliś E., Hartikainen H., The effects of short-term selenium stress on Polish and Finnish wheat seedlings-EPR, enzymatic and fluorescence studies**,** J. Plant Physiol., 169, 275–284, 2012.
7. Łabanowska M., Bidzińska E., Pietrzyk S., Juszczak L., Fortuna T., Błoniarczyk K., Influence of copper catalyst on the mechanism of carbohydrate radicals generation in oxidized potato starch**,** Carbohydr. Polym., 85, 775–785, 2011.

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.

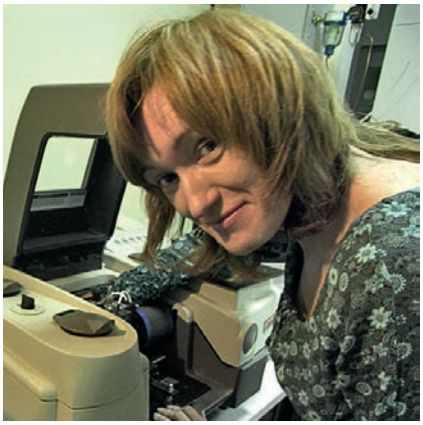
More information: http://www.chemia.uj.edu.pl/~lasocha

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 $ZnMo_2O_7$ˇ$5H_2O$”, 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.

Tomasz Łojewski

Dr habil, PhD

Research profile

Analytical chemistry; Cultural heritage objects; Conservation; Cellulose

My research interests are in the area of conservation chemistry. I mainly concentrate on the application of analytical methods to studies of cultural heritage objects and on the development of innovative methods of their active and passive conservation. The Paper Degradation Laboratory (which I supervise) was established to provide scientific support for the Paper Clinic, the Jagiellonian University center for mass-scale deacidification of paper-based materials. Over time, our interests have developed from paper degradation studies to other materials, such as silk, wool, colorants, as well as to conservation treatments, such as disinfection.

The Paper Degradation Laboratory utilizes numerous analytical techniques, including chromatography (GC/MS, DESI-MS, SEC with MALS detection, capillary electrophoresis), spectroscopy (XRF, UV/VIS, FTIR, Raman), imaging techniques (optical microscopy, hyperspectral imaging), and techniques dedicated to studies of paper, its mechanical properties, color and aging processes.

Current research projects are focused on three main areas: (1) micro-scale accelerated aging of colored materials (paper, textiles), where we develop a novel, non-destructive method of light-stability testing, (2) application of low-temperature non-thermal plasma for disinfection of paper-based documents, and (3) design of biostatic packaging material for artworks, for which we utilize nanosilver-containing paper fillers.

Within my activity I organized a post-graduate course in '*Modern analytical techniques in conservation of cultural heritage objects*', chiefly addressed to art-conservators and conservation scientists. I also teach a course in '*Paper degradation*' at the Academy of Fine Arts in Kraków.

Selected publications

1. Łojewski T., Thomas J., Gołąb R., Kawałko J., Łojewska J., Light ageing with simultaneous colorimetry via fibre optics reflection spectrometry, Rev. Sci. Instrum., 82, art. no. 076102, 2011.
2. Łojewski T., Zięba K., Kołodziej A., Łojewska J., Following cellulose depolymerization in paper: comparison of size exclusion chromatography techniques, Cellulose, 18, 1349–1363, 2011.
3. Łojewski T., Zięba K., Łojewska J., Size exclusion chromatography and viscometry in paper degradation studies. New Mark-Houwink coefficients for cellulose in cupriethylenediamine, J. Chromatogr. A, 1217, 6462–6468, 2010.
4. Łojewski T., Łojewska J., Zięba K., Knapik A., Bagniuk J., Lubańska A., Evaluating paper degradation progress. Cross-linking between chromatographic, spectroscopic and chemical results, Appl. Phys. A, 100, 809–821, 2010.

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, he took up PhD studies at the University of Erlangen-Nürnberg, Germany, in the group of Professor Horst Kisch. 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. Since 2011 he has been employed as a Jagiellonian University Professor. His research interests include heterogeneous photocatalysis (especially TiO_2 photosensitization and activation of small molecules at wide bandgap semiconductors), photocatalytic detoxification and disinfection, as well as photoelectrochemistry of semiconductors. He was awarded the Albert Weller Prize, the Staedtler Prize, in addition to the fellowships from the Foundation for Polish Science and *Polityka* magazine. In 2010 he received the Prime Minister's Prize for the habilitation thesis.

At present he carries out several research projects funded by the Foundation for Polish Science (FNP; TEAM project "Activation of small molecules in photocatalytic systems"), 7th Framework Programme (FP7; "Fourth generation photocatalysts: nano-engineered composites for water decontamination in low-cost paintable photoreactors"), Ministry of Science (MNiSW; IDEAS Plus project "Surface engineering for control of primary processes at irradiated semiconductors") and the National Science Centre (NCN; OPUS project "Photocatalysis under visible light – Ti^{IV} complexes as TiO_2 photosensitizers").
More information: www.fotokataliza.pl or www.photocatalysis.eu.

Selected publications

1. Jańczyk A., Krakowska E., Stochel G., Macyk W., Singlet oxygen photogeneration at surface modified titanium dioxide, J. Am. Chem. Soc., 128, 15574–15575, 2006.
2. 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.
3. Gawęda S., Podborska A., Macyk W., Szaciłowski K., Nanoscale optoelectronic switches and logic devices, Nanoscale, 1, 299–316, 2009.
4. Stochel G., Brindell M., Macyk M., Stasicka Z., Szaciłowski K., Bioinorganic Photochemistry (book, 398 pages), Wiley, 2009.
5. Kuncewicz J., Ząbek P., Kruczała K., Szaciłowski K., Macyk W., Photocatalysis involving a visible light-induced hole injection in a chromate(VI)-TiO_2 system, J. Phys. Chem. C, 116, 21762–21770, 2012.
6. Buchalska M., Kuncewicz J., Świętek E., Łabuz P., Baran T., Stochel G., Macyk W., Photoinduced hole injection in semiconductor-coordination compound systems, Coord. Chem. Rev., 257, 767–775, 2013.

Katarzyna Madej

Dr habil, PhD

Research profile

Sample preparation techniques; Clinical and forensic toxicological analysis; Food analysis

My scientific work mainly concerns development and optimization of analytical procedures for medicaments, especially psychotropic drugs, in biological samples. My research interests include clinical and forensic toxicology, biological sample preparation techniques, and development of chromatographic and capillary electrophoretic methods. Recently, my scientific area has been extended to food analysis in relation to eco-toxicological problems.

I defended my doctoral thesis entitled "Development of computer-aided potentiometric multicomponent titration methods" at the Faculty of Chemistry, Jagiellonian University. In 1992–1999 I was employed in the Institute of Forensic Research in Kraków, since 1995 as the Institute expert for organic poisons and non-volatile compounds. In 1999 I began my scientific career at the Faculty of Chemistry, Jagiellonian University as an assistant, and from 2002 as an assistant professor. In 2013 I completed habilitation in the field of "Analytical investigations of the selected psychotropic drugs in body fluids for forensic and clinical purposes", which I defended at the Faculty of Pharmacy, Jagiellonian University Medical College.

Selected publications

1. Madej K., Parczewski A., Kała M., HPLC/DAD screening method for selected psychotropic drugs in blood, Toxicol. Mech. Meth., 13, 121–127, 2003.
2. Madej K., Kała M., Woźniakiewicz M., Analysis of promazine in biological fluids by HPLC and MECC with spectrophotometric detection in two cases of fatal poisoning, Probl. Forensic Sci., 56, 17–22, 2003.
3. Madej K., Woźniakiewicz M., Kała M., Method for screening and quantification of seven phenothiazines in whole blood samples by non-aqueous capillary electrophoresis, Chromatographia, 61, 259–263, 2005.
4. Madej K., Kochana J., Woźniakiewicz M., Study of SPE conditions for determination of tricyclic antideressants present in body fluids, J. Liq. Chromatogr. R. T., 30, 185–198, 2007.
5. Madej K., Microwave-assisted and cloud-point extraction in determination of drugs and other bioactive compounds, TrAC-Trend Anal. Chem., 28, 436–446, 2009.
6. Madej K., Biedroń A., Garbacik A., Study of separation and extraction conditions for five neuroleptic drugs by an LLE-HPLC-DAD method in human plasma, J. Liq. Chromatogr. R. T., 32, 3025–3037, 2009.
7. Madej K., Persona K., Nizio M., Application of micelle-mediated extraction in preparation of body fluids for HPLC-DAD screening of acidic and neutral drugs, Acta Chromatogr., 25, 97–110, 2013.

Wacław Makowski

Dr habil, PhD

Research profile

Porosity; 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 porous structure and surface of adsorbents and catalysts by means of thermodesorption of probe molecules. A considerable achievement in this field was a successful application of the quasi-equilibrated thermodesorption of n-alkanes as a method for characterization of micro- and mesoporous materials, along with their mesopore size distribution.

Other fields of interests cover adsorption of organic compounds on porous solids as well as catalytic applications of zeolites and other porous solids.

Selected publications

1. Makowski W., Majda D., Temperature programmed equilibrated desorption of n-hexane as a tool for characterization of the microporous structure of zeolites, Thermochim. Acta, 412, 131–137, 2004.
2. 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.
3. 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.
4. 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.
5. 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. Mater., 120, 257–262, 2009.
6. Mańko M., Gil B., Janus R., Kuśtrowski P., Makowski W., Characterization of the porosity and surface chemistry of mesoporous silicas by quasi-equilibrated thermodesorption of 1-butanol and n-nonane, Thermochim. Acta, 511, 82–88, 2010.
7. Makowski W., Mlekodaj K., Majda D., Characterization of acidic zeolite catalysts by thermodesorption and cracking of n-nonane, Micropor. Mesopor. Mater., 166, 137–143, 2013.
8. Mańko M., Chal R., Trens P., Minoux D., Gérardin C., Makowski W., Porosity of micromesoporous zeolites prepared via pseudomorphic transformation of zeolite Y crystals, Micropor. Mesopor. Mater., 170, 243–250, 2013.
9. Makowski W., Mańko M., Dudek A., Mlekodaj K., Application of quasi-equilibrated thermodesorption of hexane and cyclohexane for characterization of porosity of zeolites and ordered mesoporous silicas, Adsorption, 2013, in press.

Artur Michalak

Professor of Chemistry, Dr habil, PhD

Research profile

Theoretical chemistry; Modeling of catalytic processes; Chemical bonding

The *Molecular Modeling of Catalytic Processes* group (Prof. A. Michalak, Dr. M. Mitoraj, Dr. M. Srebro, Ł. Piękoś, M. Brela, K. Dyduch) specializes in theoretical studies covering various aspects of theoretical chemistry, organometallic chemistry, and catalysis. Recent scientific interest has been focused on:
(i) Theoretical description of chemical bonding. In particular, new sets of orbitals have been proposed: *Natural Orbitals for Chemical Valence* (NOCV), and *Localized Orbitals from Bond-Order Operator* (LOBO),
(ii) DFT modeling of the polymerization processes catalyzed by TM complexes, and 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,
(iii) Relationship between the catalyst structure and activity,
(iv) Influence of the catalyst structure on the polyolefin branching and mictrostructure,
(v) DFT modeling of the ammonia borane dehydrogenation catalyzed by the organometallic complexes in the context of hydrogen storage materials.

Prof. Artur Michalak is a co-author of 80 publications, including seven book chapters; total number of citations > 1600; Hirsch-index is 25.

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. Kim S.-K., Han W.-S., Kim T.-J., Kim T.-Y., Nam S.W., Mitoraj M., Piękoś Ł., Michalak A., Hwang S.-J., Kang S.O., Palladium catalysts for dehydrogenation of ammonia borane with preferential B-H activation, J. Am. Chem. Soc., 132, 9954–9955, 2010.
6. 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.
7. 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 and ionic coordination 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*: Dr. Michał Poźniczek, Dr. Zofia Kluz, Dr. Małgorzata Krzeczkowska, Dr. Paweł Broś, Dr. Paweł Bernard, Karol Dudek, MSc.

II. As a member of the *Phase Transitions Research* team, 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 temperatures range of 10–400 K are performed by means of complementary methods, such as inelastic and *quasi*-elastic neutron scattering, IR and Raman spectroscopies, NMR, X-ray and neutron diffraction, thermogravimetry and DSC. *Co-workers*: Prof. Edward Mikuli, Dr. Elżbieta Szostak, Dr. Łukasz Hetmańczyk, Dr. Joanna Hetmańczyk, Dr. Natalia Górska.

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

Selected publications

1. Szostak E., Migdał-Mikuli A., Hołderna-Natkaniec K., Gwoździk-Bujakowski R., Kaczor A., Phase transitions and molecular reorientations in $[Mn(OS(CH_3)_2)_6](ClO_4)_2$ studied by proton magnetic resonance and Raman spectroscopy, J. Coord. Chem., 65, 2732–2742, 2012.
2. Górska N., Inaba A., Migdał-Mikuli A., Phase behaviour of crystalline $[Cr(DMSO)_6](BF_4)_3$ studied by adiabatic calorimetry and FT-IR spectroscopy, Vibr. Spectr., 62, 222–228, 2012.
3. Hetmańczyk J., Hetmańczyk Ł., Migdał-Mikuli A., Mikuli E., Wesełucha-Birczyńska A., Raman light scattering, infrared absorption and differential scanning calorimetry studies of the phase transition and vibrational & reorientational dynamics of H_2O ligands and ClO_4^-anions in $[Ba(H_2O)_3](ClO_4)_2$, J. Raman Spectrosc., 43, 1118–1125, 2012.
4. Szostak E., Migdał-Mikuli A., Kaczor A., Nitek W., Low-temperature phase transition in $[Mn(OS(CH_3)_2)_6](ClO_4)_2$ studied by single crystal X-ray diffraction, infrared absorption and Raman scattering spectroscopes, Spectrochim. Acta A, 79, 1179–1186, 2011.
5. Hetmańczyk J., Hetmańczyk Ł., Migdał-Mikuli A., Mikuli E., Natkaniec I., Phase transition in $[Ca(NH_3)_6](ClO_4)_2$ studied by neutron scattering methods and far infrared spectroscopy, J. Alloy. Compd., 509, 6545–6550, 2011.
6. Migdał-Mikuli A., Bernard P., Preparation of support materials for specialist courses for chemistry students, Ann. Polish Chem. Soc., 362–365, 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, and ionic coordination crystals; Orientational and structural glasses

Scientific interests of the *Phase Transitions Research* team (Professor Edward Mikuli (Head), Professor Anna Migdał-Mikuli, Łukasz Hetmańczyk, PhD, Elżbieta Szostak, PhD, Joanna Hetmańczyk, PhD, Natalia Górska, PhD, Kacper Drużbicki, PhD) 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 (10–400 K) are performed by means of complementary methods, such as inelastic and *quasi*-elastic neutron scattering, infrared absorption and Raman scattering spectroscopies, nuclear magnetic resonance, X-ray and neutron diffraction, thermogravimetry, adiabatic 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. Dołęga D., Mikuli E., Inaba I., Górska N., Hołderna-Natkaniec K., Nitek W., Calorimetric, spectroscopic and structural investigations of phase polymorphism in $[Ru(NH_3)_6](BF_4)_3$. Part I, J. Solid State Chem., 197, 429–439, 2013.
2. Drużbicki K., Mikuli E., Zalewski S., Ossowska-Chruściel M.D., Chruściel J., Wróbel S., Czerwiec J., Complementary studies of mesomorphic properties in a novel antiferroelectric liquid crystalline thiobenzoate, Spectrochim. Acta, 105, 424–438, 2013.
3. Hetmańczyk Ł., Górska N., Hetmańczyk J., Mikuli E., Natkaniec I., Phase transitions in $[Co(NH_3)_6](ClO_4)_3$ investigated by neutron scattering methods, Chem. Phys., 412, 1–6, 2013.
4. Mikuli E., Migdał-Mikuli A., Majda D., Thermal decomposition of polycrystalline $[Ni(NH_3)_6](NO_3)_2$, J. Therm. Anal. Cal., DOI: 10.1007/s10973-012-2640-8.
5. Hetmańczyk J., Hetmańczyk Ł., Migdał-Mikuli A., Mikuli E., Wesełucha-Birczyńska A., Raman light scattering, infrared absorption and differential scanning calorimetry studies of the phase transition and vibrational & reorientational dynamics of H_2O ligands and ClO_4^- anions in $[Ba(H_2O)_3](ClO_4)_2$, J. Raman Spectrosc., 43, 1118–1125, 2012.
6. Drużbicki K., Mikuli E., Kocot A., Ossowska-Chruściel M.D., Chruściel J., Zalewski S., Complex vibrational analysis of an antiferroelectric liquid crystal based on solid state oriented quantum chemical calculations and experimental molecular spectroscopy, J. Phys. Chem. A, 116, 7809–7821, 2012.
7. Drużbicki K., Kocot A., Mikuli E., Ossowska-Chruściel M.D., Chruściel J., Temperature-dependent infrared spectroscopy studies of a novel antiferroelectric thiobenzoate, J. Phys. Chem. B., 116, 11332–11343, 2012.

Jacek Młynarski

Professor of Chemistry, Dr habil, PhD

Research profile

Asymmetric synthesis; Metal complexes; Organocatalysis, Carbohydrate synthesis

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, 2008.

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. Synthesis of novel chiral ligands for aqua-asymmetric carbon-carbon and carbon-hydrogen bond formations (designing of water-compatible chiral Zn- and Fe-based chiral Lewis acids).
2. Towards enzyme mimics: direct aldol reaction in water promoted by chiral Zn(II) complexes and by small organic molecules.
3. Synthesis of carbohydrates, glycosides and bioactive natural products.

More information: www.jacekmlynarski.pl

Selected publications

1. Woyciechowska M., Forcher G., Buda S., Mlynarski J., General switch in regioselectivity in the Mukaiyama aldol reaction of silyloxyfuran with aldehydes in aqueous solvents, Chem. Commun., 48, 11029–11031, 2012.
2. Gut B., Mlynarski J., Biomimetic organocatalytic synthesis of carbohydrates, Chem. Soc. Rev., 41, 587–596, 2012.
3. Paradowska J., Pasternak M., Gut B., Gryzło B., Mlynarski J., Direct asymmetric aldol reaction inspired by two types of aldolases: Water compatible organocatalysts and Zn^{II} complexes, J. Org. Chem., 77, 173–187, 2012.
4. Mlynarski J., Paradowska J., Catalytic asymmetric aldol reactions in aqueous media, Chem. Soc. Rev., 37, 1502–1511, 2008.
5. Paradowska J., Stodulski M., Mlynarski J., Direct catalytic asymmetric aldol reactions assisted by zinc complex in the presence of water, Adv. Synth. Catal., 239, 1041–1046, 2007.
6. Jankowska J., Paradowska J., Rakiel B., Mlynarski 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.
7. Jankowska J., Mlynarski J., Zn(pybox)-Complex catalyzed asymmetric aqueous Mukaiyama-aldol reactions, J. Org. Chem., 71, 1317–1321, 2006.

Roman F. Nalewajski

Professor of Chemistry, Dr habil, PhD

Research profile

Theoretical chemistry; Quantum chemistry; Chemical physics; Theory of chemical reactivity; Information theory of molecular systems; Communication theory of the chemical bond; Entropic principles; Quantum entropy/information

Current scientific interests: (i) Density Functional Theory (ii) Bond orders; (iii) Applications of Information Theory in extracting chemical interpretation of molecular electronic structures: entropic principles and molecular equilibria, information origins of the chemical bond, locating chemical bonds and determining their multiplicities, information measures reflecting probability and current densities in molecules.

Selected publications

1. Nalewajski R.F., Exploring molecular equilibria using quantum information measures, Ann. Phys. Leipzig, 2013, in press.
2. Nalewajski R.F., Entropic concepts in electronic structure theory, Found. Chem., 2013, in press.
3. Nalewajski R.F., Use of Harriman's construction in determining molecular equilibrium states, J. Math. Chem., 51, 369-381, 2013.
4. Nalewajski R.F., Information-theoretic multiplicities of chemical bond in Shull's model of H_2, J. Math. Chem., 51, 7-20, 2013.
5. Nalewajski R.F., Gurdek P., Bond-order and entropic probes of the chemical bonds, Struct. Chem., 23, 1383-1398, 2012.
6. Nalewajski R.F., Direct (through-space) and indirect (through-bridge) components of molecular bond-multiplicities, Int. J. Quantum Chem., 112, 2355-2370, 2012.
7. Nalewajski R.F., Entropy/information descriptors of the chemical bonds revisited, J. Math. Chem., 49, 2308-2329, 2011.
8. Nalewajski R.F., On interference of orbital communications in molecular systems, J. Math. Chem., 49, 806-815, 2011.
9. Nalewajski R.F., Through-space and through-bridge components of chemical bonds, J. Math. Chem., 49, 371-392, 2011.
10. Nalewajski R.F., Szczepanik D., Mrozek J., Bond differentiation and orbital decoupling in the orbital communication theory of the chemical bond, Adv. Quant. Chem., 61, 1-48, 2011.
11. Nalewajski R.F., Electronic-geometric coupling in model reactive system, J. Math. Chem., 48, 752-775, 2010.
12. Nalewajski R.F., de Silva P., Mrozek J., Use of non-additive Fisher information in probing the chemical bonds, THEOCHEM, 954, 57-74, 2010.

Books

1. Nalewajski, R.F., *Information Theory of Molecular Systems*, Elsevier, Amsterdam, 2006.
2. Nalewajski, R.F., *Information Origins of the Chemical Bond*, Nova, New York, 2010.
3. Nalewajski, R.F., *Perspectives in Electronic Structure Theory*, Springer, Heidelberg, 2012.

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. 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 at: www.chemia.uj.edu.pl/zespol.php?id=10019.

Selected publications

1. Plewa A., Yusa S.-I., Szuwarzyński M., Szczubiałka K., Morishima Y., Nowakowska,M., J. Med. Chem., 55, 8712–8720, 2012.
2. Drozd D., Szczubiałka K., Łapok Ł., Skiba M., Patel H., Gorun S.M., Nowakowska M., Appl. Catal. B-Environ., 125, 35–40, 2012.
3. Kępczyński M., Jamróz D., Wytrwał M., Bednar J., Rząd E., Nowakowska M., Langmuir, 28, 676–688, 2012.
4. Kopeć M., Kruk T., Zapotoczny S., Laschewsky A., Holdcroft S., Mac M., Nowakowska M., J. Mat. Chem., 22, 140–145, 2012.
5. Golonka M., Bulwan M., Nowakowska M., Testera, A.M., Rodríguez-Cabello J.C., Zapotoczny S., Soft Matter, 7, 9402–9409, 2012.
6. Kamieński K., Płonka M., Ciejka J., Szczubiałka K., Nowakowska M., Lorkowska B., Korbut R., Lach R., J. Med. Chem., 54, 6586–6596, 2011.
7. Kępczyński M., Kumorek M., Stępniewski M., Róg T., Kozik B., Jamróz D., Bednar J., Nowakowska M., J. Phys. Chem. B, 114, 15483–15494, 2010.
8. Jamróz D., Kępczyński M., Langmuir, 26, 15076–15079, 2010.
9. Wybrańska K., Niemiec W., Szczubiałka K., Nowakowska M., Morishima Y., Chem. Mat., 22, 5392–5399, 2010.
10. Niemiec W., Zapotoczny S., Szczubiałka K., Laschewsky A., Nowakowska M., Langmuir, 26, 11915–11920, 2010.
11. Kamiński K., Szczubiałka K., Zazakowny K., Lach R., Nowakowska M., J. Med. Chem., 53, 4141–4147, 2010.
12. Kamiński K., Zazakowny K., Szczubiałka K., Nowakowska M., Biomacromolecules, 9, 3127–3132, 2008.
13. Kępczyński M., Lewandowska J., Romek M., Zapotoczny S., Ganachaud F., Nowakowska M., Langmuir, 23, 7314–7320, 2007.

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. Andruniów T., Pawlikowski M., Zgierski M.Z., Density functional study of absorption 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., Gawroński 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 (postdoctoral at 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, Ring-Opening Polymerization (with R.H. Grubbs), Elsevier, 2012, and several chapters in monographs and encyclopedias. His papers were cited over 6000 times with h = 43.

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, in 2004 he was elected to the IUPAC Bureau, and in 2010 to the IUPAC Executive Committee. 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, JASP Personal Medal in Japan, and Śniadecki Medal of the Polish Chemical Society.

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. He has been elected to the German Nordrhein Akademie der Wissenschaften, and in 2012 to the Polish Academy of Art and Sciences.

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; Polariton; 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 (1981, 1982, 1993), National Research Council, Ottawa, Canada; Visiting Professor: Ulm University, Germany (1983), Université Louis Pasteur, Strasbourg, France (1985, 1990); Visiting Fellow, 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. B, 71, art. no. 235205, 2005.
7. Brocławik E., Góra A., Liguzinski P., Petelenz P., Witek H.A., Quantum chemical modelling of electrochromism of tungsten oxide films, J. Chem. Phys., 124, art. no. 054709, 2006.
8. Zapotoczny S., Rymarczyk-Machał M., Stradomska A., Petelenz P., Nowakowska M., Aggregates of naphthalene chromophores in poly(vinylalcohol)-graft-poly(winyl-naphthalene) pseudomicelles, J. Phys. Chem. B, 111, 10088–10094, 2007.
9. Petelenz P., Kulig W., Intra-band relaxation of Frenkel excitons in sexithiophene crystals, Phys. Rev. B, 80, art. no.115127, 2009.
10. Stradomska A., Kulig W., Slawik M., Petelenz P., Intermediate vibronic coupling in charge transfer states: Comprehensive calculation of electronic excitations in sexithiophene crystal, J. Chem. Phys., 134, art. no. 224505, 2011.

Wojciech Piekoszewski

Professor of Medical Sciences, Dr habil, PhD

Research profile

Toxicology; Pharmacokinetics; Addictive substances; Metals; Mass spectrometry; 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); Research Director of the Institute of Forensic Research (1997–2007).

Current position: Head of the *Toxicological and Pharmaceutical Analysis* Group in the Department of Analytical Chemistry, and Head of the *Laboratory of High-resolution Mass Spectrometry* in the Regional Laboratory of Physicochemical Analysis and Structural Research at the Faculty of Chemistry, Jagiellonian University.

Major scientific interest: determination of drugs of abuse in biological materials; application of alternative materials in toxicological analysis; application of lipidomics study in metabolic diseases and psychiatric disorders; application of mass spectrometry (Matrix-Assisted Laser Desorption/Ionization Time-Of-Flight Mass Spectrometry – MALDI-TOF/TOF MS) in proteomics, lipidomics and mapping of drug, protein and lipid distribution in different tissues.

Selected publications

1. 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.
2. 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.
3. Grela A., Turek A., Piekoszewski W., Application of Matrix-Assisted Laser Desorption/ Ionization Time-of-Flight Mass Spectrometry (MALDI-TOF MS) in Alzheimer's disease, Clin. Chem. Lab. Med., 50, 1297–1304, 2012.
4. Przybylowicz A., Chęsy P., Herman M., Parczewski A., Walas S., Piekoszewski W., Examination of distribution of trace elements in hair, fingernails and toenails as alternative biological materials. Application of chemometric methods, Cent. Eur. J. Chem., 10, 1590–1599, 2012.
5. Majcherczyk J., Kulza M., Seńczuk-Przybyłowska M., Florek E., Jawien, W., Piekoszewski W., Influence of tobacco smoke on the pharmacokinetics of citalopram and its enantiomers, J. Physiol. Pharmacol., 63, 95–100, 2012.
6. Gawlikowski T., Gomolka E., Piekoszewski W., Jawien W., Undas A., Acute CO poisoning is associated with impaired fibrinolysis and increased thrombin generation, Basic Clin. Pharmacol. Toxicol., Doi: 10.1111/bcpt.12042, 2013.

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 p-bond in the vitamin B_{13} complex, *cis*-ammine(orotato)copper(II): theoretical and vibrational spectroscopy studies, J. Phys. Chem. B, 113, 8158–8169, 2009.
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.

Edyta Proniewicz

Dr habil, PhD

Research profile

Vibrational spectroscopy; Surface-enhanced Raman spectroscopy; Neurotransmitters; Hemoproteids; Phosphonate analogues of amino acids and peptides

My scientific interests concentrate on solving questions of molecular structure and adsorption mechanism at metal/liquid interfaces of biologically active compounds (neurotransmitters, hemoproteids, phosphonate analogues of amino acids and peptides, pharmaceuticals, and food additives), their synthetic models, and bioinorganic complexes. Experimental techniques used in my studies are mainly: Raman spectroscopy, resonance Raman spectroscopy, surface enhanced (resonance) Raman spectroscopy, time resolved resonance Raman spectroscopy, infrared spectroscopy, and electron absorption spectroscopy. Theoretical investigations are based on *ab initio* and density functional theory.

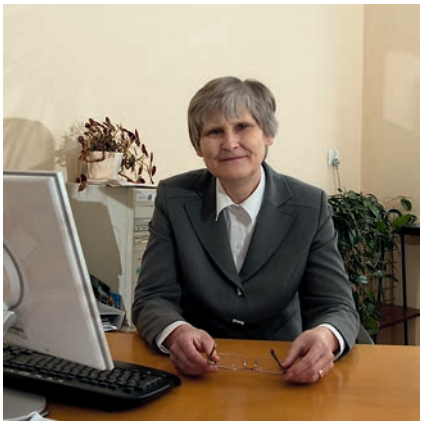
I am the author or co-author of 82 publications, amongst which 65 (IF = 183,946) were published in the international journals listed by the Institute of Scientific Information in Philadelphia. Please see http://www.chemia.uj.edu.pl/~podstawk/ang/index.htm for my scientific achievements.

Selected publications

1. Podstawka-Proniewicz E., Ignatjev I., Niaura G., Proniewicz L.M., Phe-MetNH_2 terminal bombesin subfamily peptides: Potential induced changes in adsorption on Ag, Au, and Cu electrodes monitored by SERS, J. Phys. Chem. C, 116, 4819–4200, 2012.
2. Proniewicz E., Skołuba D., Kudelski A., Sobolewski D., Kim Y., Prahl A., Proniewicz L.M., B_2 Bradykinin receptor antagonists: Adsorption mechanism onto electrochemically roughened Ag substrate, J. Raman Spectrosc., 44, 205–211, 2013.
3. Pienpinijtham P., Proniewicz E., Kim Y., Ozaki Y., Lombardi J.R., Proniewicz L.M., Molecular orientation of neurotensin and its single-site mutants on colloidal silver surface: SERS studies, J. Phys. Chem. C, 116, 16561–16572, 2012.
4. Ignatjev I., Proniewicz E., Proniewicz L.M., Niaura G., Effect of potential on temperature-dependent SERS spectra of neuromedin B on Cu electrode, Phys. Chem. Chem. Phys., 15, 807–815, 2013.
5. Proniewicz E., Pienpinijtham P., Ozaki Y., Kim Y., Andrzejak M., Proniewicz L.M., Influence of backbone length and synthetic mutations on orientation of neurotensin fragments adsorbed onto a colloidal silver surface: SERS studies, J. Raman Spectrosc., 44, 55–62, 2013.

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. and. 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., Enantio-differentiation by ^{1}H NMR spectroscopy (dirhodium method) – selectivity of oxygen functionalities, Nat. Prod. Commun., 3, 339–344, 2008.

Barbara Sieklucka

Professor of Chemistry, Dr habil, PhD

Research profile

Multifunctional molecular inorganic materials; Coordination chemistry

Our current research interest is in multifunctional molecular inorganic materials. We focus our work on the crystal engineering of new polynuclear coordination compounds with spin-carriers. The aim of the research is to obtain novel highly-structured functional magnetic materials based on polynuclear cyanido-bridged coordination compounds. The research is focused on the development of rational design and synthetic strategies, which will impart specific functionalities, such as dynamics, sorption, magnetism, photomagnetism, porosity, chirality, non-linear optics etc., to target materials, with the ultimate goal of achieving multifunctionality and efficient engineering of the nanospace within the crystal network. This fundamental research has the clear application perspective.

Bibliographic data: 91 publications in peer reviewed journals. Sum of times cited: 1631. h-index 23; 27 research grants.

Current international co-operation: Prof. Corine Mathoniere, l'Université de Bordeaux-1, Institut de Chimie de la Matière Condensée de Bordeaux, France ; Prof.Shin-ichi Ohkoshi, School of Chemistry, University of Tokyo, Japan.

Selected publications

1. Pinkowicz D., Podgajny R., Gaweł B., Nitek W., Łasocha W., Oszajca M., Czapla M., Makarewicz M., Bałanda M., Sieklucka B., Double switching of a magnetic coordination framework through intraskeletal molecular rearrangement, Angew. Chem. Int. Ed., 50, 3973–3977, 2011.
2. Chorąży S., Nakabayashi K., Imoto K., Mlynarski J., Sieklucka B., Ohkoshi S., Conjunction of chirality and slow magnetic relaxation in the supramolecular network constructed of crossed cyano-bridged Co^{II}-W^{V} molecular chains, J. Am. Chem. Soc., 134, 16151–16154, 2012.
3. Pinkowicz D., Rams M., Nitek W., Czarnecki B., Sieklucka B., Evidence for magnetic anisotropy of $[Nb^{IV}(CN)_8]^{4-}$ in pillared-layered Mn_2Nb framework showing spin-flop transition, Chem. Commun., 48, 8323–8325, 2012.
4. Nowicka B., Korzeniak T., Stefańczyk O., Pinkowicz D., Chorąży S., Podgajny R., Sieklucka B., The impact of ligands upon topology and functionality of octa-cyanidometallate-based assemblies, Coord. Chem. Revs., 256, 1946–1971, 2012.
5. Podgajny R., Chorąży S., Nitek W., Marszałek B., Rams M., Majcher A.M., Żukrowski J., Kapusta C., Sieklucka B., Co-NC-W and Fe-NC-W electron-transfer channels for thermal bistability in trimetallic $\{Fe_6Co_3[W(CN)_8]_6\}$ cyanido-bridged cluster, Angew. Chem. Int. Ed., 52, 896–900, 2013.
6. Chorąży S., Nakabayashi K., Ozaki N., Pełka R., Fic T., Mlynarski J., Sieklucka B., Ohkoshi S., Thermal switching between blue and red luminescence in magnetic chiral cyanido-bridged Eu^{III}-W^{V} coordination helices, RSC Advances, 3, 1065–1068, 2013.

Zbigniew Sojka

Professor of Chemistry, Dr habil, PhD

Research profile

Materials and Surface Chemistry; Heterogeneous Catalysis; Molecular Modeling; Spectroscopy; Electron Paramagnetic Resonance and Transmission Electron Microscopy techniques

Appointments: Vice-Dean for Education and European Integration (2005–2008); Vice-Dean for Research and Cooperation (2008–2012); JU Senate Member; Head of the Inorganic Chemistry Department (2003–2009); Head of the Catalysis and Solid State Group

The research interest of our group focuses on synthesis, spectroscopic characterization and reactivity studies of nanostructured and porous inorganic materials, which are functionalized with transition metal ions for guiding surface reactions along specific pathways. In our methodology we combine various spectroscopic techniques, high resolution electron microscopy with quantum chemical calculations, including ab initio thermodynamic and microkinetic modeling. We design and investigate model systems of controlled electronic and magnetic structure with tunable redox properties for establishing quantitative structure-property-function relationships, and elucidation of catalytic reaction mechanisms with particular insights into dynamics of interfacial spin and charge transfer processes.

Selected publications

1. 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.
2. 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.
3. Maurelli S., Ruszak M., Witkowski S., Pietrzyk P., Chiesa M., Sojka Z, Spectroscopic CW-EPR and HYSCORE investigations of Cu^{2+} and O_2^- species in copper doped nanoporous calcium aluminate ($12CaO{\cdot}7Al_2O_3$), Phys. Chem. Chem. Phys., 12, 10933-10941, 2010.
4. Zasada F., Piskorz W., Stelmachowski P., Kotarba A., Paul J.-F., Płociński T., Kurzydłowski K.J., Sojka Z, Periodic DFT and HR-STEM studies of surface structure and morphology of cobalt spinel nanocrystals. Retrieving 3D shapes from 2D images, J. Phys. Chem. C, 115, 6423-6432, 2011.
5. Piskorz W., Zasada F., Stelmachowski P., Diwald O., Kotarba A., Sojka Z., Computational and experimental investigations into N_2O decomposition over MgO nanocrystals from thorough molecular mechanism to ab initio microkinetics, J. Phys. Chem. C, 115, 22451–22460, 2011.
6. Pietrzyk P., Podolska,K., Mazur T., Sojka Z., Heterogeneous binding of dioxygen: EPR and DFT evidence for side-on nickel(II)-superoxo adduct with unprecedented magnetic structure hosted in MFI zeolite, J. Am. Chem. Soc., 133, 19931–19943, 2011.
7. Godlewski S., Tekiel A., Piskorz W., Zasada F., Prauzner-Bechcicki J.S., Sojka Z., Szymonski M., Supramolecular ordering of PTCDA molecules: The key role of dispersion forces in an unusual transition from physisorbed into chemisorbed state, ACS Nano, 6, 8536–8545, 2012.

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 in ferroics; Structure-pharmacological activity relationship for compounds showing anti-arrhythmic and/or adrenergetic properties; Structure of minerals.

Research associates and their topics: Dr. Anna Krawczuk – Optical properties of crystalline organic materials from electron density; Dr. Marlena Gryl – Crystal engineering of materials with prospective non-linear optical properties in terms of experimental charge density; Tomasz Seidler, MSc – *In silico* studies of linear and non-linear optical properties in crystal engineering of functional materials, Marzena Suder, MSc, Eng. – Living cell interactions with the surface of mineral-apatite plates of specified crystallographic orientation.

Selected publications

1. Krawczuk A., Stadnicka K., J. Phys. Chem. A, 116, 9759–9768, 2012.
2. Nowicka B., Stadnicka K., Nitek W., Rams M., Sieklucka B., CrystEngComm, 14, 6559–6564, 2012.
3. Szklarzewicz J., Stadnicka K., Inorg. Chim. Acta, 392, 131–136, 2012.
4. Ostrowska K., Piegza E., Rąpała-Kozik M., Stadnicka K., Eur. J. Org. Chem., 19, 3636–3646, 2012.
5. Jabłońska-Wawrzycka A., Stadnicka K., Masternak J., Zienkiewicz M., J. Mol. Struct., 1012, 97–104, 2012.
6. Szlachcic P., Kolek P., Uchacz T., Stadnicka K., J. Mol. Struct., 1012, 87–96, 2012.
7. Wesełucha-Birczyńska A., Zelek S., Stadnicka K., Vib. Spectrosc., 60, 124–128, 2012.
8. Dudek L., Grolik J., Kaźmierska A., Szneler E., Eilmes A., Stadnicka K., Eilmes J., Tetrahedron Lett., 52, 3597–3601, 2011.
9. Gryl M., Krawczuk-Pantula A., Stadnicka K., Acta Crystallogr. B, 67, 144–154, 2011.
10. Jabłońska-Wawrzycka A., Barszcz B., Stadnicka K., J. Therm. Anal. Calorim., 101, 463–469, 2010.
11. Trzewik B., Seidler T., Brocławik E., Stadnicka K., New J. Chem., 34, 2220–2228, 2010.
12. Hryniewicz K., Stadnicka K., Adamski A., Pattek-Janczyk A., J. Coord. Chem., 63, 977–987, 2010.
13. Janik A., Bukowska M., Jamroży K., Stadnicka K., Struct. Chem., 20, 699–707, 2009.
14. Gryl M., Krawczuk A., Stadnicka K., Acta Crystalogr. B, 64, 623–632, 2008.

Grażyna Stochel

Professor of Chemistry, Dr habil, PhD

Research profile

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

Appointments: Dean (since 2008); Head of the *Coordination and Bioinorganic Physicochemistry* Group; Head of Laser Photolysis Laboratory; Humboldt Foundation Fellow; Visiting Professor at the Orleans University; Member of Chemistry Committee of PAS.

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; (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 scientific 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 (www.bioinorg.nanophotonics.pl).

Selected publications

1. Pilch M., Dudkowiak A., Jurzyk B., Łukasiewicz J., Susz A., Stochel G., Fiedor L., Molecular symmetry determines the mechanism of a very efficient ultrafast excitation-to-heat conversion in Ni-substituted chlorophylls, Biochim. Biophys. Acta-Bioenergetics, 1827, 30–37, 2013.
2. Mazuryk O., Kurpiewska K., Lewiński K., Stochel G., Brindell M., Interaction of apo-transferrin with anticancer ruthenium complexes NAMI-A and its reduced form, J. Inorg. Biochem., 116, 11–18, 2012.
3. Silva E.F.F., Serpa C., Dąbrowski J.M., Monteiro C.J.P., Formosinho S.J., Stochel G., Urbanska K., Simões S., Pereira M.M., Arnaut L.G., Mechanisms of singlet-oxygen and superoxide-ion generation by porphyrins and bacteriochlorins and their implications in photodynamic therapy, Chem. Eur. J., 16, 9273–9286, 2010.
4. Orzeł Ł., Jańczyk A., Brindell M., Stopa G., Stochel G., New trends in the application of laser flash photolysis – case studies, J. Coord. Chem., 63, 2695–2714, 2010.
5. Szaciłowski K., Macyk W., Stochel G., Light-driven OR and XOR programmable chemical logic gates, J. Am. Chem. Soc., 128, 4550–4551, 2006.
6. Szaciłowski K., Macyk W., Drzewiecka-Matuszek A., Brindell M., Stochel G., Bioinorganic photochemistry: Frontiers and mechanisms, Chem. Rev., 105, 2647–2694, 2005.

Books

1. Stochel G., Stasicka Z., Brindell M., Macyk M., Szaciłowski K., Bioinorganic Photochemistry, 398 pages, Wiley, 2009.
2. van Eldik R., Stochel G. (editors), Advances in Inorganic Chemistry, Inorganic Photochemistry, Vol. 63, Elsevier, Academic Press, 464 pages, 2011.

Grzegorz D. Sulka

Dr habil, PhD

Research profile

Nanotechnology; Nanostructured materials fabrication and characterization; Anodization of valve metals; Electrochemistry; Electrocatalysis; Electrochemical sensors; Corrosion of metals and alloys

Research interest is focused on fabrication, characterization, and applications of nanostructured materials:

- Anodization of valve metals. Synthesis of nanoporous metal oxides by self-organized anodization of aluminum, titanium, zirconium and tin.
- Fabrication and characterization of nanowire arrays. Home-made anodic aluminum oxide (AAO) templates are used for fabrication of nanoporous thin metallic films and nanowires with different dimensions (diameter and length), shapes (Y-branched, multi-level branched, nanoporous, or diameter modulated), and compositions (alloyed, composite or multilayered). Polymers, semiconductors and metals nanowire arrays are fabricated by electrodeposition or electropolymerization.
- Applications of nanostructured materials. Fabricated nanostructured materials are used as electrochemical sensors, materials for electrocatalysis, photoelectrocatalysis, thermoelectrics and functional nanoporous materials for biomedical implants.

More information is available at: http://www.chemia.uj.edu.pl/~sulka/

Selected publications

1. Zaraska L., Kurowska E., Sulka G.D., Jaskuła M., Template assisted fabrication of tin and antimony based nanowire arrays, Appl. Surf. Sci., 258, 9718–9722, 2012.
2. Sulka G.D., Hnida K., Distributed Bragg reflector based on porous anodic alumina fabricated by pulse anodization, Nanotechnology, 23, art no. 075303, 2012.
3. Sulka G.D., Zaraska L., Stępniowski W.J., Anodic porous alumina as a template for nanofabrication, in: Encyclopedia of Nanoscience and Nanotechnology, 2nd Edition, Nalwa H.S. (Ed.), American Scientific Publishers 2011, vol. 11, pp. 261–349.
4. Sulka G.D., Brzózka A., Liu L., Fabrication of diameter-modulated and ultrathin porous nanowires in anodic aluminum oxide templates, Electrochim. Acta, 56, 4972–4979, 2011.
5. Sulka G.D., Jóźwik P., Electrochemical behavior of Ni_3Al-based alloys in NaOH, Intermetallics, 19, 974–981, 2011.
6. Sulka G.D., Kapusta-Kołodziej J., Brzózka A., Jaskuła M., Fabrication of nanoporous TiO_2 by electrochemical anodization, Electrochim. Acta, 55, 4359–4367, 2010.
7. Sulka G.D., Brzózka A., Zaraska L., Jaskuła M., Through-hole membranes of nanoporous alumina formed by anodizing in oxalic acid and their applications in fabrication of nanowire arrays, Electrochim. Acta, 55, 4368–4376, 2010.

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 (i) surface engineering of nanocrystalline materials, (ii) microwave-assisted synthesis and (photo)electrochemistry of wide band gap semiconductors, (iii) information processing at molecular level, and (iv) molecular nanoelectronics. Recently his research is mainly focused on construction of photoelectrochemical neuromorphic systems (so called artificial neurons) and artificial neural networks utilizing coupled chemical reactions and diffusion.

Selected publications

1. Szaciłowski K., *Infochemistry – Information Processing at the Nanoscale*, Wiley 2012, ISBN-13: 978-0470710883.
2. Gawęda S., Kowalik R., Kwolek P., Macyk W., Mech J., Oszajca M., Podborska A., Szaciłowski K., Nanoscale digital devices based on the photoelectrochemical photocurrent switching effect: Preparation, properties and applications, Isr. J. Chem., 51, 36–55, 2011.
3. Podborska A., Oszajca M., Gawęda S., Szaciłowski K, Nanoparticles with logic and numeracy: towards 'computer-on-a-particle' optoelectronic devices, IET Circ. Dev. Syst. 5, 103–114, 2011.
4. Oszajca M., McCall K.L., Robertson N., Szaciłowski K., Photocurrent switching effects in TiO_2 modified with ruthenium polypyridine complexes, J. Phys. Chem. C, 115, 12187–12195, 2011.
5. Lewandowska K., Szaciłowski K., Molecular photodiode and two-channel demultiplexer based on the [60]fullerene-porphyrin tetrad, Austr. J. Chem., 64, 1409–1413, 2011.
6. Kwolek P., Oszajca M., Szaciłowski K., Catecholate and 2,3-acenediolate complexes of d^0 ions as prospective materials for molecular electronics and spintronics, Coord. Chem. Rev., 256, 1706–1731, 2012.

Janusz Szklarzewicz

Professor of Chemistry, Dr habil, PhD

Research profile

Inorganic chemistry; Coordination compounds; Transition metals; Reaction mechanisms; Ligand activation; Catalysis; Metallopharmaceutics; MOF

Professor J. Szklarzewicz is Head of the *Coordination Chemistry* group in Department of Inorganic Chemistry. The main research interest of the group is the synthesis and investigation of new metal complexes (mainly with molybdenum, tungsten, iron and vanadium), notably, those with rare coordination numbers and/or symmetry. In the investigation of the structure and properties of the compounds, both experimental and theoretical methods (quantum chemical calculations) are used. Other research topics include the transition metal spin states, kinetics and mechanisms of inorganic reactions (activation of small molecules, metal assisted catalysis in synthesis of new organic compounds). The latter topic is intensively investigated as a source of organic molecules produced in simple one step reactions ("green chemistry").

The metal complexes are also studied in the context of their practical applications as metallopharmaceutics (for example as insulin mimetic compounds, antidepressants, etc.), as mezoporous materials (as part of metal-organic-framework complexes), and as catalysts for organic synthesis.

Selected publications

1. Szklarzewicz J., Samotus A., Kanas A., Polyhedron, 11, 1733–1740, 1986.
2. Samotus A., Szklarzewicz J., Coord..Chem.Rev., 125, 63–74, 1993.
3. Matoga D., Mikuriya M., Szklarzewicz J., Inorg. Chem., 45, 7100–7104, 2006.
4. Szklarzewicz J., Matoga D., Lewiński K., Inorg. Chim Acta., 360, 2002–2008, 2007.
5. Szklarzewicz J., Matoga D., Niezgoda A., Yoshioka Y., Mikuriya M., Inog. Chem., 46, 9531–9533, 2007.
6. Szklarzewicz J., Matoga D., Kłyś A., Łasucha W., Inorg. Chem., 47, 5464–5472, 2008.
7. Szklarzewicz J., Matoga D., Owcarz M., Przybylski W., Yoshio D., Mikuriya M., Inorg. Chem. Commun., 12, 819–822, 2009.
8. Stawski T., Szklarzewicz J., Kotarba A., Stelmachowski P., Polyhedron, 28, 473–478, 2009.
9. Matoga D., Szklarzewicz J., Lewiński K., Polyhedron., 29, 94–99, 2010.
10. Radoń M., Brocławik E., Pierloot K., J. Chem. Phys. B., 114, 1518–1528, 2010.
11. Radoń M., Brocławik E., Pierloot K., J. Chem. Theory Comput., 7, 898–908, 2011.
12. Szklarzewicz J., Stadnicka K., Inorg. Chim. Acta, 393 131–136, 2012.
13. Mikuriya M., Yoshioka D., Borta A., Luneau D., Matoga D., Szklarzewicz J., Handa M., New J. Chem., 35, 1226–1233, 2011.
14. Matoga D., Szklarzewicz J., Nitek W., Polyhedron, 36, 120–126, 2012.
15. Ryniewicz A., Tomecka M., Szklarzewicz J., Matoga D., Nitek W., Polyhedron, 45, 229–237, 2012.
16. Gryboś R., Paciorek P., Szklarzewicz J.T., Matoga D., Zabierowski P., Kaze G., Polyhedron, 49, 100–104, 2013.

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^0 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.

Stanisław Walas

Dr habil, PhD

Research profile

Analytical Chemistry; Sorbents for heavy metals FIA preconcentration; Application of atomic spectrometry in a wide range of analyses

Research interests cover mainly two fields. The first one is focused on preparation of new sorbents synthesized on the basis of the ion imprinting idea, dedicated to heavy metals SPE preconcentration realized with the use of FIA technique coupled on-line with FAAS determination. The new sorbents are examined to evaluate their physical and physicochemical characteristics along with their applicability to FI-FAAS environmental analysis. The second field is directed to development of sample preparation procedures, optimization of determination conditions and application of different atomic spectrometric techniques such as FAAS, GFAAS, ICP OES, ICP MS and HG AFS in biological, medical and environmental analysis.

The area of interests also covers the utilization of ICP mass spectrometry in analysis of solid samples (mapping of biological samples or historical objects examination) with the use of laser ablation (LA).

Selected publications

1. Gawin M., Konefał J., Trzewik B., Walas S., Tobiasz A., Mrowiec H., Witek E., Preparation of a new Cd(II)-imprinted polymer and its application to determination of cadmium(II) via flow injection flame atomic absorption spectrometry, Talanta, 80, 1305–1310, 2010.
2. Gawin M., Bryłka M., Mrowiec H., Tobiasz A., Trzewik B., Wala S., Salen impregnated silica gel as a new sorbent for on-line preconcentration of cadmium(II), Int. J. Environ. Anal. Chem., 91, 484–492, 2011,
3. Filek M., Walas S., Mrowiec H., Rudolphy-Skórska E., Sieprawska A., Biesaga-Kościelniak J., Membrane permeability and micro- and macroelement accumulation in spring wheat cultivars during the short-term effect of salinity- and PEG-induced water stress, Acta Physiol. Plant., 34, 985–995, 2012.
4. Kępa M., Kozłowski T., Szostek K., Drozd A., Walas S., Mrowiec H., Stepańczaka B., Głąb H., Grupa M., Analysis of mercury levels in historical bone material from syphilitic subjects – pilot studies (short report), J. Biol. Clinic. Anthrop., 69, 367–377, 2012.
5. Tobiasz A., Walas S., Soto Hernández A., Mrowiec H., Application of multiwall carbon nanotubes impregnated with 5-dodecylsalicylaldoxime for on-line copper preconcentration and determination in water samples by flame atomic absorption spektrometry, Talanta, 96, 89–95, 2012.
6. Tobiasz A., Walas S., Landowska L., Konefał-Góral J., Improvement of copper FAAS determination conditions via preconcentration procedure with the use of salicylaldoxime complex trapped in polymer matrix, Talanta, 96, 82–88, 2012.

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, 4526–533, 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, from her graduation associated with 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-vinyl-formamide), 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 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), Cambridge University (1990, 1997), University of Munich (1990–1991), Oklahoma State University (1991–92), University of Illinois, Chicago (1982), NRC Canada (1993, 1994), Kyushu University (1995, 2011), University of Natal, South Africa (1996), IMS Okazaki (1997–98), University of Bordeaux (1999), KEK Tsukuba (2000, 2001, 2002), Tohoku University (2003), Purdue University (2004), University of Perpignan (2004), Emory University (2006), Kwansei Gakuin University (2007), Technical University of Munich (2007, 2008, 2009, 2010), University of Malaya, Kuala Lumpur (2012).

Research areas: (i) theoretical studies of hydrogen-bonded systems, water, aqueous ionic solutions and ices, (ii) quantum-mechanical calculations, (iii) theoretical studies of multi-dimensional proton tunneling, (iv) Car-Parrinello simulations.

Research staff: Marek Boczar, PhD, DSc, Łukasz Boda, PhD.

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

Selected publications

1. Witkowski A., Wójcik M., Infrared spectra of hydrogen bond. A general theoretical model, Chem. Phys., 1, 9–16, 1973.
2. Wójcik M.J., Theory of the infrared spectra of the hydrogen bond in molecular crystals, Int. J. Quant. Chem., 10, 747–760, 1976.
3. Wójcik M.J., Buch V., Devlin J.P., Spectra of isotopic ice mixtures, J. Chem. Phys., 99, 2332–2344, 1993.
4. Wójcik M.J., Boda Ł., Boczar M., Theoretical study of proton tunneling in the excited state of tropolone, J. Chem. Phys., 130, 164306, 2009.
5. Wójcik M.J., Kwiendacz J., Boczar M., Boda Ł., Ozaki Y., Theoretical and spectroscopic study of hydrogen bond vibrations in imidazole and its deuterated derivative, Chem. Phys., 372, 72–81, 2010.
6. Brela M., Stare J., Pirc G., Sollner-Dolenc M., Boczar M., Wójcik M.J., Mavri J., Car-Parrinello simulation of the vibrational spectrum of a medium strong hydrogen bond by two-dimensional quantization of the nuclear motion: Application to 2-hydroxy-5-nitrobenzamide, J. Phys. Chem. B, 116, 4510–4518, 2012.

Szczepan Zapotoczny

Dr habil, PhD

Research profile

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

Szczepan Zapotoczny is a university professor, head of the *Nanoengineering of Functional Polymeric Materials* team in the Department of Physical Chemistry, and also a supervisor of the Atomic Force Microscopy (AFM) Laboratory. His current research interests focus on nanostructural polymeric materials (films, brushes) for photochemical and biomedical applications as well as on hybrid systems containing superparamagnetic and noble metal nanoparticles. The main processes he develops are: (i) electrostatically-driven self-assemblies of charged nanoobjects (polymers, nanoparticles), and (ii) syntheses of polymer brushes performed with use of controlled radical polymerizations. In his studies that lie at the border of nanotechnology, materials science, biology and medicine, he uses AFM as the primary technique.

In his research activity he cooperates with many Polish and foreign groups on topics, such as functional polymeric coatings for biological objects, stimuli responsive brushes, and biological synthesis of silver nanoparticles.

Selected publications

1. Szuwarzyński M., Zaraska L., Sulka G.D., Zapotoczny S., Pulsatile releasing platform of nanocontainers equipped with thermally-responsive polymeric nanovalves, Chem. Mat., 25, 514–520, 2013.
2. Szpak A., Kania G., Skórka T., Tokarz W., Zapotoczny S., Nowakowska M., Stable aqueous dispersion of superparamagnetic iron oxide nanoparticles protected by charged chitosan derivatives, J. Nanoparticles Res., 15, art. no. 1372, 2013.
3. Szuwarzyński M., Kowal J., Zapotoczny S., Self-templating surface-initiated polymerization: a route to conductive brushes, J. Mat. Chem., 22, 20179–20181, 2012.
4. Kopeć M., Kruk T., Zapotoczny S., Laschewsky A., Holdcroft S., Mac M., Nowakowska M., Photoinduced electron transfer in multilayer films composed of conjugated polyelectrolyte and amphiphilic copolymer hosting electron acceptor molecules, J. Mat Chem., 22, 140–145, 2012.
5. Benetti E.M., Sui X., Zapotoczny S., Vancso G.J., Surface-grafted gel-brush/metal nanoparticle hybrids, Adv. Funct. Mat., 20, 939–944, 2010.
6. 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.
7. Zapotoczn S., Golonka M., Nowakowska M., Nanostructured micellar films formed via layer-by-layer deposition of photoactive polymer, Langmuir 24, 5868–5876, 2008.
8. Zapotoczny S., Benetti E.M., Vancs G.J., Preparation and characterization of macromolecular “hedge” brushes grafted from Au nanowires, J. Mat. Chem., 17, 3293–3296, 2007.

Emeriti Professors

Andrzej Barański

Professor of Chemistry, Dr habil, PhD

Research Profile

Chemical kinetics; Catalysis; Degradation and de-acidification of paper; Fundamentals of stoichiometry – teaching and metrology

Born 31 Oct. 1934, Vilnius; MSc 1955, PhD 1961, Habilitation 1965, Professor 1975, Full professor 1987, Emeritus 2005.

My research topics have included: properties of ammonia-CO_2-water system and synthesis of urea from CO_2 and NH_3 (1955–1975), temperature programmed desorption from gas-solid systems, e.g. ZnO-H_2 and zeolites-butenes (1970–1979), high-temperature oxidation of graphite electrodes (1982–1992), reduction of fused iron catalyst for NH_3 synthesis – the bellwether reaction in heterogeneous catalysis (1967–2000), reduction of iron ores, mainly hematite to magnetite (1985–1997), degradation and de-acidification of paper [1] (1996 to present), and fundamentals of stoichiometry (2011 to present).

In the latter field my recent article [4] was focused on criticism of the current definitions of the atomic mass unit and the mole. The expected redefinition of the mole and the kilogram ('atomic kilogram version') was briefly outlined.

Another recent field of my interest is 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 [2–3].

Author of over 100 publications and of three book chapters; Organizer and Head of the Kinetics of Heterogeneous Reactions research group (1970–2006); 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). The activity that the latter function involved, included among others: (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.

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., Gdy ważyły się losy zjednoczenia Europy, Alma Mater, Jagiellonian University, Kraków, 98, 22–27, 2007.
3. Barański A., Dokument sprzed 60 lat, CX News, Consultronix S.A., Kraków, No 1/39/2012, p. 21; see also www.cxnews.pl
4. Barański A., The atomic mass unit, the Avogadro constant, and the mole: A way to understanding, J. Chem. Educ., 89, 97–102, 2012.

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 the 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 and Wrocław University; City of Kraków medal "Cracoviae Merenti", Erazm Jerzmanowski award (PAAS), 2012.

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.

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.

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 250 papers in international journals, the number of their citations being over 2500 (h-index of 29). 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, 11760–17766 , 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. 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.
7. Brocławik E., Załucka J., Kozyra P., Mitoraj M., Datka J., New insights into charge low processes and their impact on the activation of ethene and ethyne by Cu(I), and Ag(I) sites in MFI, J. Phys. Chem., 114, 9808–9816, 2010.
8. Sadowska K., Góra-Marek K., Drozdek M., Kuśtrowski P., Datka J., Desilication of highly siliceous zeolite ZSM-5 with NaOH and NaOH/tetrabutylamine hydroxide, Micropor. Mesopor. Mat., 168, 195–205, 2013.

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 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. Dyrek K., Che M., EPR as a tool to investigate the transition metal chemistry on oxide surfaces, Chem. Rev., 97, 305–331, 1997.
4. Blennow A., Houborg K., Andersson R., Bidzińska E., Dyrek K., Łabanowska M., Phosphate positioning and availability in the starch granule matrix as studied by EPR, Biomacromolecules, 7, 965–974, 2006.
5. Błaszczak W., Bidzińska E., Dyrek K., Fornal J., Wenda E., EPR study of the influence of high hydrostatic pressure on the formation of radicals in phosphorylated potato starch, Carbohydr. Polym., 82, 1256–1263, 2010.
6. Szostak M.M., Chojnacki H., Piela K., Okwieka-Lupa U., Bidzińska E., Dyrek K., Helical superstructure and charged polarons contributions to optical nonlinearity of 2-methyl-4-nitroaniline crystals studied by resonance Raman, electron paramagnetic resonance, circular dichroism spectroscopies and quantum chemical calculations, J. Phys. Chem. A, 115, 7448–7455, 2011.
7. Bidzińska E., Błaszczak W., Dyrek K., Fornal J., Kruczala K., Michalec M., Rozwora M., Szczygieł J., Wenda E., Effect of phosphorylation of the maize starch on thermal generation of stable and short-living radicals, Starch/Staerke, 64, 729–739, 2012.

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 three other groups (Catalysis & Solid State Chemistry II, Industrial Catalysts & Adsorbents, Technology of Materials and Nanomaterials) and ESCA and Thermal Analyses & Calorimetry Laboratories; Former Dean of the Faculty of Chemistry; Humboldt Foundation Fellow; Five 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 250, cited 1900 times (h = 24).

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-$LiMn_2O_{4-y}S_y$ ($0 \leq y \leq 0.5$) composites, J. Power Sources, 174, 613–618, 2007.

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.

Adam Juszkiewicz

Professor of Chemistry, Dr habil, PhD

Research profile

Environmental chemistry; Environmental chemical analysis

Head of the Department of General Chemistry (1996–2012); 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. Studies on bioactive compounds and antioxidant properties of plant extracts.

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. 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.
5. Juszkiewicz A., Bartynowska-Meus Z., Kawałek M., Meus M., Łaptaś A., Wpływ oczyszczalni ścieków na jakość wód dorzecza Rudawy, Aura, 6, 12–14, 2006.
6. 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.
7. Kot M., Karcz W., Zaborska W., 5-Hydroxy-1,4-naphthoquinone (juglone) and 2-hydroxy-1,4-naphthoquinone (lawsone) influence on jack bean urease activity: elucidation of the difference in inhibition activity, Bioorg. Chem., 38, 132–137, 2010.
8. Kot M., Olech Z., Influence of 2,5-dichloro-1,4-benzoquinone on jack bean urease activity. Inhibitor effect, total reducing capacity and DPPH radical scavenging activity, Acta Biochim. Pol., 58, 627–633, 2011.
9. Olech Z., Zaborska W., A spectrophotometric assay for total garlic thiosulfinates content. Kinetic aspects of reaction with chromogenic thiols, Pol. J. Food Nutr. Sci., 62, 23–29, 2012.

Jan Najbar

Professor of Chemistry, Dr habil, PhD

Research profile

Photophysics and photochemistry of organic molecules; Photoinduced electron transfer; Supersonic jet spectroscopy; Geometry electronically excited organic molecules

Research is carried out in the field of physical chemistry related to photophysics and photochemistry of organic molecules, and to laser spectroscopy. The emphasis is on the early events that follow light absorption. The research topics include: (i) spin-orbit interactions in molecules and weak molecular complexes, (ii) ultrafast electron transfer processes and solvation dynamics, (iii) theory of multistep charge separation phenomena, (iv) spectroscopy of jet-cooled organic molecules, (v) laser induced fluorescence.

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.

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.

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

Degrees in chemistry: MSc 1959; PhD 1966; Habilitation 1980, all at the Jagiellonian University; Professor of Chemistry 2000.

Appointments: Polish Academy of Sciences 1959–1974 (assistant, assistant professor); Jagiellonian University 1975 (assistant professor, associate professor, full professor); Post doctoral fellowship at van't Hoff Laboratory, University of Utrecht, Holland, 1968–1969; Head of Department of Physical Chemistry and Electrochemistry, 1992–2006, Head of research group of Physical Chemistry of Surfaces, 1981-present.

Research areas: (i) properties of adsorption monolayers at the water/air interface (composition and interactions in mixed adsorption films, thermodynamic and electric properties of molecules at the free surface of water), (ii) properties of insoluble monolayers spread on aqueous subphases, particulary those leading to the application of Langmuir monolayers as a model of biomembranes. Earlier research topics included application of the interfacial cell to potentiometric titration in non-conducting solvents, stability of suspensions in aqueous and non-aqueous media and properties of free black films.

Selected publications

1. Paluch M., Electrical properties of free surface of water and aqueous solutions, Adv. Colloid Interface Sci., 84, 27–45, 2000.
2. Wydro P., Paluch M., Surface properties of cationic-nonionic surfactants system, J. Colloid Interface Sci., 245, 75–79, 2004.
3. Korchowiec B., Paluch M., Corvis Y., Rogalska E., A Langmuir film approach to elucidating interaction in lipid membranes: 1,2-dipalmitoyl-sn-glycero-3-phosphoethanolamine/ cholesterol/ metal cation systems, Chem. Phys. Lipids, 144, 127–136, 2006.
4. Gzyl-Malcher B., Paluch M., Studies on the lipid interactions in mixed Langmuir monolayers, Thin Solid Films, 516, 8865–8872, 2008.
5. Makyła K., Paluch M., The linoleic acid influence on molecular interactions in the model of biological membrane, Colloids Surf. B, 71, 59–66, 2009.

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.

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, with the aim of supporting the Faculty and promoting it in Poland and abroad.

Chairpersons:

Wacław Makowski, Dr habil, Chairman of the Executive Board

Barbara Krajewska, Dr habil, Vice-Chairman of the Executive Board

Prof. Maria Nowakowska, Chairman of the Supervisory Board

Prof. Piotr Petelenz, Vice-Chairman of the Supervisory Board

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- performing chemical analyses and other scientific studies,
- publishing scientific and educational materials,
- organizing training courses for candidates, students and teachers,
- organizing scientific and educational conferences, symposia and meetings.

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