INSTITUTE OF PHYSICAL CHEMISTRY
POLISH ACADEMY OF SCIENCES

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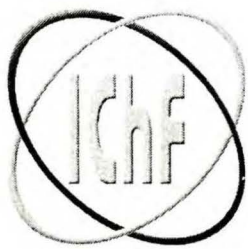

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Contents

Historical outline

The Institute of Physical Chemistry of the Polish Academy of Sciences was founded on March 19, 1955 by the resolution of the Presidium of the Government of the People's Republic of Poland. The scientific goals of the Institute were described as follows: "The activity of the Institute of Physical Chemistry covers research on current issues in the field of physical chemistry which are important from the point of view of the development of chemical sciences and demands of the national economy".

The Institute of Physical Chemistry was the first research institute dedicated to chemical sciences in Poland. During the first period of the existence of the Institute the main task was to prepare scientific staff that would be able to undertake fundamental research in the field of physical chemistry and to provide them with the appropriate laboratories and equipment. The development of the scientific staff was possible due to the fact that the scientists in the research institute were free from teaching duties obligatory in universities and therefore were able to concentrate their activity solely on the development of science.

The first employees of the Institute included: members of the Polish Academy of Sciences: Professor W. Świętosławski, Professor St. Bretsznajder, Professor B. Kamieński, Professor M. Śmiałowski, Professor W. Trzebiatowski; professors: W. Kemula, St. Minc, K. Gumiński, J. Kamecki; four associate professors (J. Berak, Z. Szklarska-Śmiałowska, J. Wojciechowska, J. Minczewski) and auxiliary scientific workers including: 12 assistant professors, 24 assistants and 15 technicians.

Pursuant to the Statute of the Institute seven scientific departments were established:

I. Department of Structural Research (Head: Prof. Dr Włodzimierz Trzebiatowski) in Wrocław - investigation of structure of fire resistant materials, semiconductors, metal alloys and contact catalizers.

II. Department of Physicochemical Analytical Methods (Prof. Dr Wiktor Kemula) – elaboration of fast methods of control of raw materials and products by means of potentiometry, polarography, chromatography, spectrochemistry, etc.

III. Department of Physical Chemistry of Basic Organic Raw Materials (Prof. Dr. Wojciech Świętosławski) – elaboration of physicochemical characterization of organic raw materials and their products, and search for ways to separate multicomponent mixtures, like *e.g.* pitches, prapitches, rock-oil, *etc.*

IV. Department of Physical Chemistry of Surface Phenomena (Prof. Dr. Bogdan Kamieński) in Kraków, with a laboratory in Lublin (Prof. Dr. A. Waksmundzki) – elaboration of the theory of flotation for separation and enrichment of minerals and raw materials, elaboration of contact processes, research in the field of adsorption and ion exchange.

V. Department of Physical Chemistry of Electrode Processes (Prof. Dr. Michał Śmiałowski) – research on mechanism of cathode and anode processes as well as on catalysis and corrosion.

VI. Department of Electrochemistry (Prof. Dr. Stefan Minc) – elaboration of fundamentals of electrolysis in aqueous and non-aqueous solutions, and in molten salts, research on contact potentials and structure of electrolytes.

VII. Department of Physicochemical Fundamentals of Technology (Prof. Dr. Stanislaw Bretsznajder) with a laboratory in Wrocław (Prof. Dr. W. Bobrownicki) – elaboration of fundamental problems of engineering and construction of chemical apparatuses and unitary technological processes.

The first Director of the Institute and at the same time Chairman of its Scientific Council was Professor Wojciech Świętosławski, the vice-Director at that time was Professor Michał Śmiałowski. After retirement of Professor Świętosławski in 1960, the next Directors were: Professor Michał Śmiałowski (1960–1973), Professor Wojciech Zielenkiewicz (1973–1990), Professor Jan Popielawski (1990–1992), Professor Janusz Lipkowski (1992–2003), Professor Aleksander Jabłoński (2003–).

Based on the text of Professor W. Zielenkiewicz written for the chronicle on the 50th anniversary of IChF PAN of PAS.

Research areas

The present scientific profile of the Institute of Physical Chemistry is strongly linked with modern directions in physical chemistry and chemical physics. The research work covers a wide range of physicochemical disciplines and is carried out in 10 departments. The main topics presently studied at the Institute are:

- supramolecular chemistry, structure and properties; X-ray structure determinations, separation techniques, sorption/desorption processes, surface aggregation (Prof. J. Lipkowski, Dr. K. Suwińska, Dr. R. Luboradzki, Dr. A. Bielejewska, Dr. M. Asztemborska); supramolecular synthesis (Assoc. Prof. M. Pietraszkiewicz);
- thermodynamics, thermochemistry and biocalorimetry (Prof. W. Zielenkiewicz); thermodynamics of liquids (Assoc. Prof. J. Gregorowicz); development of transitiometry as a tool for study EOS and phase transitions (Assoc. Prof. S. Randzio)
- physical chemistry of solid state and surface, examined by various electron spectroscopy techniques (Prof. A. Jabłoński) and scanning tunneling microscopy techniques (Dr. R. Nowakowski);
- photophysics and photochemistry of organic molecules, involving spectrally and time resolved laser techniques (Prof. J. Waluk, Prof. Z. R. Grabowski, Prof. A. Grabowska, Prof. K. Rotkiewicz, Assoc. Prof. J. Herbich, Assoc. Prof. A. Kapturkiewicz, Assoc. Prof. J. Sepioł, Assoc. Prof. J. Dobkowski, Assoc. Prof. R. Kołos);
- studies of interaction of gas phase (mainly hydrogen) with surface of metals and alloys, especially during metal-semiconductor transition which can occur in the bulk (Prof. R. Duś);
- preparation and characterisation of highly dispersed mono- and bimetallic catalyst systems, aided by X-ray diffraction analysis (Prof. Z. Karpiński, Prof. J. Pielaszek, Assoc. Prof. Assoc. Prof. Jerzy Zieliński); structure of nanocrystalline systems modeling and experiment (Assoc. Prof. J. Pielaszek, Dr. Z. Kaszkur, Dr. B. Mierzwa); catalysis for environmental problems (Prof. Z. Karpiński, Prof. J. Pielaszek);
- statistical mechanics applied to soft matter (Prof. R. Hołyst, Prof. J. Stecki, Prof. A. Ciach, Dr. A. Poniewierski);
- electrochemistry (Prof. J. Taraszewska, Prof. Z. Borkowska, Assoc. Prof. P. Żółtowski, Prof. W. Kutner, Assoc. Prof. M. Opałło); elektrochemical oxidation of gasous fuels (Prof. L. Rostwo-Suski);
- theory of chemical kinetics (including periodical reactions), aided by computer simulations (Assoc. Prof. A. Kawczyński, Prof. J. Górecki);
- quantum theory of the solid and the molecule: the density functional theory, the chemical reactivity indices (Prof. A. Holas, Dr M.Cinal, Dr R. Balawender); theory of the magnetic thin films and the 2D crystalline systems (Prof. S. Olszewski, Dr M.Cinal, Dr T. Roliński); hydrocarbons with unusual spatial structure, molecular modeling and NMR studies of cyclodextrins, fullerenes and nanotubes (Prof. H. Dodziuk);
- corrosion, surface modification and hydrogen in metals (Prof. J. Flis, Prof. E. Łunarska, Prof. T. Zakroczymski, Prof. M. Janik-Czachor);
- kinetics and mechanism of chain reactions in homogeneous/heterogeneous systems, as related to sulphur dioxide transformations in the environment: physico-chemical fundamentals of desulphurization processes; atmosphere chemistry including impacts of organic and inorganic scavengers of sulphoxy radicals; interaction between these radicals and bioorganic compounds (Prof. W. Pasiuk-Bronikowska, Dr T. Bronikowski, Dr K.J. Rudziński, Dr J. Ziajka);

- physical chemistry of metal-hydrogen systems, including synthesis of novel materials under high pressure conditions and research of their properties; determination of EOS and search of pressure induced phase transitions in hydrides (Prof. B. Baranowski, Assoc. Prof. S. M. Filipek, Assoc. Prof. M. Tkacz).

Technological section of the Institute, the CHEMIPAN Laboratories (headed by Marek Cieślak, M. Sc.), develops and commercially manufactures fine and specialty chemicals and specialised products for agriculture and pharmacy, including pheromones ("biological traps" for woods and crop protection) and new drugs.

The Institute employees publish about 300 original papers each year.

Educational activities

In addition to research, IChF PAN also has an educational mission, both at the post-graduate and under-graduate levels.

The School for post-graduate studies was established in 1965. It provides training at the post-graduate level in the fields of both physical and theoretical chemistry. Since 1965, 224 Ph.D. degree have been thus conferred. The main topics for Ph.D. study presently include:

- electrochemistry, corrosion protection, electrocatalysis and studies of metal-solution interfaces;
- the physical chemistry and structure of supramolecular complexes and their applications;
- the physical and chemical properties of solid state surfaces and heteregenous catalysis as probed by photoelectron spectroscopy;
- photochemistry, photophysics and molecular spectroscopy
- chemical and process kinetics
- thermodynamics, thermochemistry and calorimetry
- the physico-chemical applications of statistical physics
- the quantum chemistry of solids and their surfaces
- mass spectrometry and the chemistry of gas phase molecular ions

The Institute was one of co-founders of the College of Science launched in 1993 (at present a part of the Cardinal Stefan Wyszyński University). More than 30 per cent of IPCh research workers are also involved in educational activities within the College at the under-graduate level. The Institute also collaborates with the Departments of Chemistry at the Warsaw University and Technical Warsaw University. Accordingly, research workers from IPCh deliver advanced courses at under-graduate level and supervise M.Sc. theses at their facilities. In addition the Institute provides equipment for advanced student exercises, and common research projects are thus undertaken.

I. Department of Physical Chemistry of Solids

Head: Associate Professor Stanisław Filipek

The scientific staff of the Department has a long-time experience in the scope of high pressure techniques with the use of gaseous media (particularly hydrogen/deuterium), synthesis of new hydrides and study of their physicochemical properties. The Department is in possession of the equipment which is unique in the world and allows to obtain results not available with the other methods.

It concerns in particular:

- piston-cylinder apparatus for pressures (in gaseous hydrogen/deuterium) to 3 GPa generated in relatively large volumes with simultaneous heating up to 1000°C,
- diamond anvils loaded with initially compressed hydrogen and allowing to generate pressures up to 20 GPa.

The equipment is gradualy developed in order to increase the available range of pressures and temperatures. A construction of an apparatus to compress gaseous oxygen in the possibly wide range of pressures is also planned.

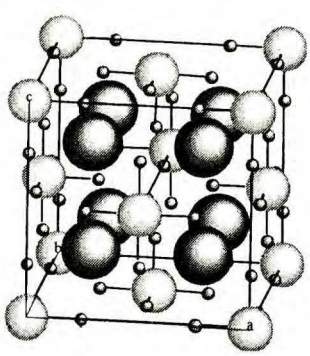
The objects of research will mainly include metal-hydrogen(deuterium) systems, particularly intermetallic compounds. Recent works have resulted in the discovery of a number of new hydrides in intermetallic compounds of the Laves phase type (*e.g.* $ErFe_2H_5$, YFe_2H_5, $ZrFe_2H_3$, $ZrCo_2H_2$, YMn_2H_6 and relevant deuterides). These hydrides (except from $ZrCo_2H_2$) are stable in normal conditions; especially it concerns YMn_2H_6 with a crystal structure dramatically reconstructed in comparison with the initial C15 structure. The new structure corresponds to the compound K_2PtCl_6 with partial disorder and may be expressed as $[YMn]MnH_6$. It is the first time such hydride has been obtained from the Laves phase.

We expect to obtain more novel hydrides; we are going to study their properties taking into account their practical applications as well (storage of hydrogen, separation of hydrogen isotopes, electrodes in hydride batteries or fuel cells).

Another research topic, started already in 1975, is the study of influence of hydrostatic pressures on the properties of metal hydrides (including hydrides of rear earths, selected alloys and intermetallic compounds). This study will aim at the determination of equation of state and search for a possibility pressure induced phase transitions. We have already observed (partly with the participation of foreign partners) phase transitions in alkali metal hydrides, in *fcc* manganese hydride, some rare earths hydrides and in hydrides newly obtained on the basis of Laves phases.

We are also going to continue the study of electronic properties of hydride phases, including low temperature range.

Further development of very fruitful cooperation is planned with Polish and foreign partners, especially from France, Taiwan, Japan, Israel, Russia and Ukraine.



Structure of the newly discovered hydride/deuteride YMn_2D_6 with the highest concentration of hydrogen/deuterium in the intermetallic compound YMn_2. As a result of treatment with deuterium, the Y and Mn atoms were radically rearranged what caused that the new structure differs fundamentally from the initial Laves Phase C15. The new hydride is highly stable and its chemical bonds have different character than in the hydrides that have been known in this system so far.

The Specialised Laboratory working in the structure of the Department is going to continue its production of pressure apparatuses for Polish and foreign customers.

Stanisław Filipek, Associate Professor

M.Sc., 1962 – Department of Metallurgy of Non-Ferrous Metals, Academy of Mining and Metallurgy in Kraków

M.A. – Japanese Studies, Warsaw University

Ph.D., 1978 – Institute of Physical Chemistry, Warsaw

D.Sc., 1991 – Institute of Physical Chemistry, Warsaw

Education and training:

1962/3 – Post-Graduate Course in Application of Nuclear Energy and Isotopes, Warsaw University

1975–76, 1989, 1997, 1998 Tokyo Institute of Technology, Tokyo, Japan

1988 – University of Munich, Germany

1998 – Science University of Tokyo, Tokyo, Japan

1988/2004 – CNRS Laboratory of Chemical Metallurgy and Spectroscopy of Rare Earth, Paris, France

2000/2006 – Taiwan National University, Taipei

Professional affiliation:

- Polish Chemical Society,
- AIRAPT – International Association for the Advancement of High Pressure Science and Technology, Member of Steering Committe

Research areas:

1. Physico-chemical investigations with application of high pressures, especially:
- syntheses of new materials; pressure induced phase transitions; equation of state
- structural, thermodynamic, electronic and magnetic properties of hydrides
2. Construction and improvement of high pressure instruments.

Selected papers

1. Baranowski B. and Filipek S.M., "Synthesis of Metal Hydrides" in: B.Baranowski and J. Jurczak (Eds) "High Pressure Chemical Synthesis" Elsevier Science Publishers, Amsterdam, Oxford, New York, Tokyo, pp. 55–100 (1989).
2. Filipek S.M., Sawaoka A.B., "Progress in the Very High Hydrogen Pressure Techniques", Kooatsu Gijutsu (JHPI), **Vol. 30**, (6) s. 43–49 (1992).
3. Filipek S.M., "Thermoelectric Power of (NiMn)–H and (NiCo)-H Systems". *Polish J. Chem.*, **71**, 1777–1786 (1997).
4. Filipek S.M., Sugiura H., Skoskiewicz T., "Pressure Induced Phase Transformations in the Mn-H and Mn-H/N" AIRAPT-17 Proc. Science and Technology of High Pressure (Murli H. Manghnani, William J. Nellis and Malcolm F. Nicol Eds.) Universities Press, Hyderabad, India p. 550–554 (2000).
5. Dorogova M., Hirata T., Filipek S.M. and Bala H., "Synthesis of a hexagonal hydride phase of $ZrCr_2H_x$ (x=5.75) under high hydrogen pressure", *J. Phys. Cond. Matter*, **14**, (44) 11151 (2002).
6. Paul-Boncour V., Bouree-Vigneron F., Filipek S.M., Marchuk I., Jacob I., Percheron-Guegan A., "Neutron Diffraction Study of ZrM_2D_x deuterides (M=Fe, Co)", *J. Alloys Comp.*, **356–357**, 69–72 (2003).
7. Paul-Boncour V., Filipek S.M., Marchuk I., Andre G., Bouree F., Wiesinger G., Percheron-Guegan A., "Structural and magnetic properties of $ErFe_2D_5$ studied by neutron diffraction and Moessbauer spectroscopy", *J. Phys., Condens. Matter.*, **15**, 4349–4359 (2003).
8. Dorogova M., Hirata T., Filipek S.M., Hydrogen-induced volume changes in $ZrCr_2$ and pseudobinary compounds of $ZrCr_2$, $ZrMn_2$ and ZrV_2, Phys. Stat. Sol. (a) **1**, 38–42 (2003).
9. Sugiura H., Marchuk I., Paul-Boncour V., Percheron-Guegan A., Kitazawa T., Filipek S.M., "Pressure induced phase transitions and EOS of several Laves phases", *J. Alloys Comp.*, **356–357**, 32 (2003).
10. Sugiura H., Paul-Boncour V., Percheron-Guégan A., Marchuk I., Hirata T., Filipek S.M., Dorogova M., High Pressure Studies of YMn_2 Laves Phase and its Deuterides, *J. Alloys Comp.*, **367**, 230 (2004).
11. Chien-Yuan Wang, Valerie Paul-Boncour, Chia-Cheng Kang, Ru-Shi. Liu, Filipek S.M., Dorogova M., Marchuk I., Toshiya Hirata, Annick Percheron-Guegan, Hwo-Shuenn Sheu, Ling-Yun Jang, Jin-Ming Chen, and Hung-Duen Yang, "New YMn2D6 Deuteride synthesized under high pressure of gaseous Deuterium", *Sol. St. Comm.*, **130**, 815 (2004).

Total number of publications: 97 (including 10 publications on Polish-Japanese relations)

Bogdan Baranowski, Professor Emeritus

M.Sc., 1951 – Department of Chemistry, University of Wrocław
Ph.D., 1956 – Institute of Physical Chemistry, Warsaw
Professor, 1964 – Institute of Physical Chemistry, Warsaw

Educating and training:

1958, 1959–60, 1970's, 1980's – Université Libre de Bruxelles, Brussels, Belgium
1965 – Institute of Atomic and Molecular Physics, Amsterdam, The Netherlands
1971–72 – Bergakademie, Freiberg, Germany
1975–2001 short stays, 1985 Jubileum Profesorship – Institute of Physics, Technical University, Göteborg, Sweden
1984, 1986 – Max Planck Institut für Festkörperforschung, Stuttgart, Germany
1987–1988 – University of Belfast, Northern Ireland

Professional affiliations:

- Polish Academy of Sciences (1973)
- Polish Chemical Society (1951, president 1974–79, honorary member 1987, honorary president 1997)
- International Association for Advancement of High Pressure Science and Technology (AIRAPT) (1975, president 1989–93)
- Deutsche Akademie der Naturforscher "Leopoldina" (1976)
- Warsaw Learned Society (1981)
- Society for Advancement of Science and Arts (TPKN) (1981)
- National Ukrainian Academy of Sciences (1994)
- Committee on Chemical Sciences of Polish Academy Sciences (1981, chairman 1981–83)
- International Academy of Sciences (1986)
- Deutsche Bunsen Gesellschaft für Physikalische Chemie (1989)
- German Chemical Society (GDR) (honorary member 1990)
- Technical University, Göteborg, Sweden, dr h.c. 1993

Research areas:

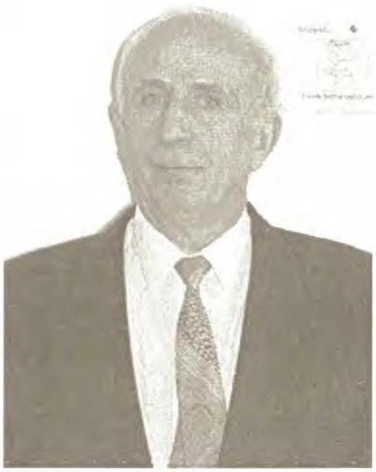
Non-equilibrium thermodynamics
High-pressure physical chemistry, especially metal-hydrogen systems

Selected papers

1. Baranowski B., "Non-equilibrium Thermodynamics in Physical Chemistry" (in Polish); PWN, Warszawa 1974; "Nicht-Gleichgewichts-Thermodynamik in der physikalischen Chemie", VEB Deutscher Verlag für Grundstoffindustrie, Leipzig (1975).
2. Baranowski B., "Metal-Hydrogen Systems at High Pressures", in "Topics in Applied Physics", **29**, "Hydrogen in Metals II" (G.Alefeld and J. Voelkl, Eds.), Springer Verlag, 1978, pp. 157–200.
3. Baranowski B., "Dissipative Strukturen als ein energetisches Problem", *Nova Acta Leopoldina NF*, **60**, Nr 265, 91–107 (1989).
4. Baranowski B., Filipek S.M., "Synthesis of Metal Hydrides" in "High Pressure Chemical Synthesis" (J. Jurczak and B. Baranowski, Eds.), Elsevier, Amsterdam pp. 55–100 (1989).
5. Baranowski B., "Diffusion in Elastic Media with Stress Fields", in "Advances in Thermodynamics, Flow, Diffusion and Rate Processes" (S. Sieniutycz and P. Salamon, Eds.), Taylor and Francis, New York, pp. 168–199 (1992).
6. Baranowski B., "A simplified quantitative approach to the isothermal hysteresis in metallic hydrides with coherent interphases", *J. Alloys and Compounds*, **200**, 87–92 (1993).

Total number of publications: 333

Marek Tkacz, Associate Professor



M.Sc., 1970 – Department of Chemistry, Warsaw University
Ph.D., 1984 – Institute of Physical Chemistry, Warsaw
D.Sc., 1998 – Institute of Physical Chemistry, Warsaw

Education and training:

1984–1986 – Chemical Engineering Department, University of Illinois

Professional affiliations:

Polish Chemical Society (since 1974)

Research areas:

- High pressure physical chemistry
- Metal-hydrogen systems

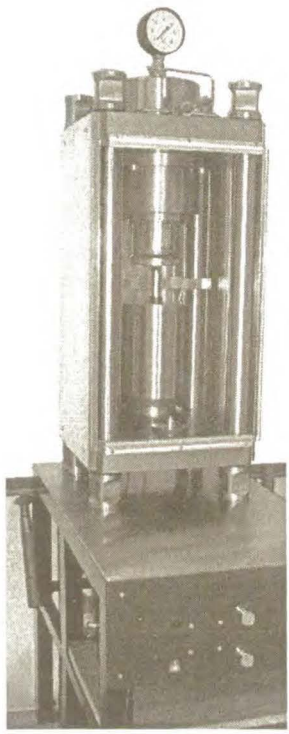
Selected papers

1. Tkacz M., Majchrzak S. and Baranowski B., "High pressure X-ray diffraction study of copper hydride" High Pressure Research, **6**, 85–89 (1990).
2. Tkacz M. and Baranowski B., "The equations of state of Pd, Ni, Cr, and their hydrides in high pressure at room temperatures", *Polish J. Chem.*, **66** 1301 (1992).
3. Tkacz M. and Baranowski B., "A pressure induced phase separation in $PdH_{0.6}$,, *Z. Phys. Chem.*, **179**, 5762 (1993).
4. Tkacz M., "High pressure studies of fcc chromium hydride", *Polish J. Chem.*, **71**, 1735–1741 (1997).
5. Tkacz M., "Novel High-Pressure Technique for Loading Diamond Anvil Cell with Hydrogen", *Polish J. Chem.*, **69**, 1205–1209 (1995).
6. Tkacz M., "High pressure studies of rhodium-hydrogen system in diamond anvil cell", *J. Chem. Phys.*, **108**, 2084–2087 (1998).
7. Burtovyy R. and Tkacz M., "High pressure synthesis of new copper hydride from elements", *Sol. St. Comm.*, **131**, 170 (2004).
8. Tkacz M. and Burtovyy R., "Decomposition of the hexagonal copper hydride at high pressure", *Sol. St. Comm.*, **132**, 37 (2004).
9. Antonov V.E., Latynin A.I. and Tkacz M., "T–P phase diagrams and isotope effects in the Mo-H/D systems", *J. Phys.; Condens. Mat.*, **16**, 8387–8398 (2004).
10. Palasyuk T. and Tkacz M., "Pressure-induced structural phase transition in rare-earth trihydrides. Part I. (GdH_3, HoH_3, LuH_3)", *Sol. St. Comm.*, **133**, 481–486 (2005).
11. Palasyuk T. and Tkacz M., "Hexagonal to cubic phase transition in YH_3 under high pressure", *Sol. St. Comm.*, **133**, 77–480 4 (2005).

Total number of publications: 63

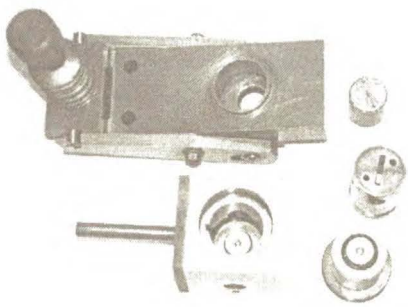
Laboratory of High Pressures

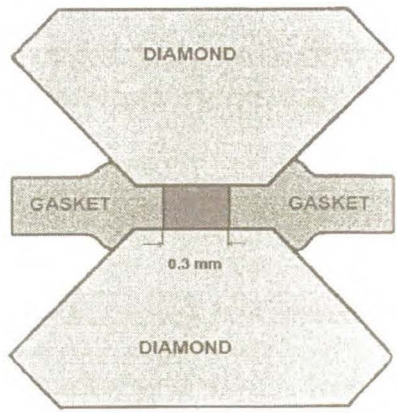
Head: Assoc. Prof. Marek Tkacz



We offer a wide variety of high pressure apparatus and techniques for the basic research in different areas of science. They are listed below.

1. Studies of different properties of materials under high pressure such as:
   - compressibility of liquids and solids
   - pressure induced phase transformations
   - transport properties.
2. High pressure chemical synthesis up to 2 GPa and 400 K.
3. X-ray diffraction studies (energy dispersive mode) in diamond anvil cells up to 40 Gpa
4. Designing and manufacturing of high pressure equipment for the liquid and gaseous media including gaseous hydrogen.
5. Hydriding and nitriding of metals and alloys up to 2 GPa





High pressure equipment available:

1. Hydraulic presses with the load ranging from 10 to 1000 tonnes.
2. High pressure chambers:
   - initial working volume – 60 ccm, pressure limit 2.5 GPa
   - initial working volume – 10 ccm, pressure limit 1.5 GPa.
3. High pressure intensifier for gaseous media including hydrogen. Pressure limit 1.2 GPa.
4. Diamond anvil cells up to 40 GPa.

Contact person:

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II. Department of Physical Chemistry of Supramolecular Complexes

Head: Professor Janusz Lipkowski

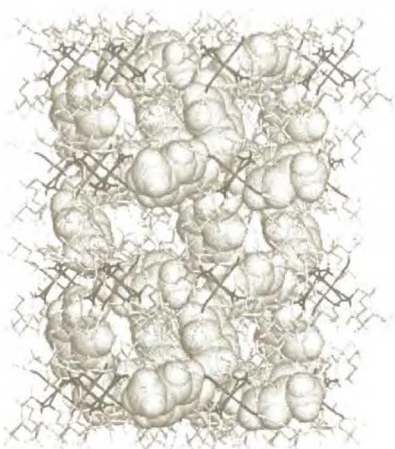
Research areas

Research work of the Department of Physical Chemistry of Supramolecular Complexes is mainly focused on the relationship between structure and selectivity of complex formation in various heteromolecular systems, where one of the components (host) is able to bind selectively and reversibly a variety of molecular species (guest). Consequently, this property may conveniently be used in the molecular processes of dynamic separation (chromatography, electrophoresis) and detection (sensors, selective electrodes, *etc.*) of different species. The Department is composed of several laboratories specialized in areas, such as X-ray structural analysis, gas and liquid chromatography, electrophoresis, molecular films, electrochemistry of sensors and chemically modified electrodes, as well as laboratories of thermodynamics and thermochemistry.

Research is directed to molecular recognition phenomena used as starting points to design systems capable of effective separation of mixtures, activation of selected chemical reactions and molecular transport. Both skeletal systems with internal cavities of molecular dimensions (organic zeolites, cyclodextrins, calixarenes and their derivatives) and systems formed by self assembly (hydrates, including hydrophobic hydrates with dominating role of non-covalent bonding and molecularly imprinted polymers) are investigated.

Development of new methods for mixture separations based on the above-mentioned processes of molecular recognition *via* inclusion complex formation are an important specialty of the Department. Separation of enantiomers is the field where a significant part of the current research projects is involved, especially characteristic is the possibility of separation by inclusion optically active compounds lacking functional groups, and, therefore, particularly difficult to separate. The analysis of enantiomeric composition of pharmaceuticals and their metabolites or natural taste-and-flavor substances or their synthetic substitutes is the example of applications of the developed analytical methods.

Structural factors play an important role in molecular inclusion processes and, consequently, most of the investigated processes have to be based on detailed structural analysis of each of the components and the complexes formed. The departmental laboratory of diffractometry is highly specialized in investigation of supramolecular complexes, which by their nature are very susceptible to the environmental changes. As a consequence, most of the measurements must be conducted in situ, *i.e.* in mother solutions. Examples are organic zeolites and hydrophobic hydrates.



The analysis of energetic effects of complexation at a supramolecular level is provided by the thermochemical group. Beyond routine characterizing the equilibrium states of the sorption-desorption processes (enthalpy, entropy), the calorimetry group has expertise in thermokinetics of these processes. What is especially important, the kinetic information is obtained from standard calorimetric measurements and kinetic parameters of the process are defined by additional analysis of thermal effects measured during experiments using original procedures elaborated by the group members.

A new approach has been developed toward the molecular architecture of Langmuir and Langmuir-Blodgett films, such as a Krick-Watson ion pairing in films of fullerene adducts with adenine, adenosine or ATP dissolved in an aqueous subphase solution or a 'two-point' binding of layers of water-insoluble metalloporphyrin derivatives with the use of simultaneous complexation of central metal ion by bidentate ligands and peripheral crown ether substituent of a porphyrin macrocycle by sodium cation in the subphase solution.

The Department has wide international collaboration and participates in the SURPHARE European Center of Excellence as well as coordinates and is a general executor of the TALES European Center of Excellence. Outstanding formal international collaboration has been established with research groups in Russia, Ukraine, Moldova, United Kingdom, Italy, France, Israel, Romania and Spain (in frames of joint research programs) and, informal but very effective collaboration, with many other laboratories in the world, *e.g.* in Japan, Taiwan, Germany, USA.

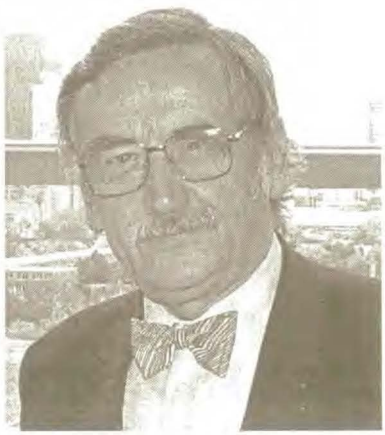
Janusz Lipkowski, Professor

M.Sc., 1965 – Faculty of Chemistry, University of Warsaw, Poland, Cum Laude

Ph.D., 1972 – Institute of Physical Chemistry, Warsaw

D.Sc., 1983 – Institute of Physical Chemistry, Warsaw

Professor, 1990 – Institute of Physical Chemistry, Warsaw



Honours and Membership of Professional Societies:

- Polish Academy of Sciences (corr. member since 1998, vice-President since April 2003)
- Polish Chemical Society (since 1970)
- Society for Propagation and Promotion of Sciences (1990)
- Societas Scientiarium Varsoviensis (member correspondent since 1992, full member since 2002, chairman of the Division of Mathematical, Physical and Chemical Sciences since 2002)
- American Crystallographic Association (since 1993)
- American Chemical Society (since 1999)
- British Crystallographic Association (since 1999)
- European Crystallographic Association (since 1999)
- Honorary Doctor, Institute of Inorganic Chemistry, Russian Academy of Sciences, Novosibirsk, Russia (1997)
- Honorary Professor, Siberian Branch of the Russian Academy of Sciences (2001)

Research areas:

- main field – crystallography
- other fields – supramolecular chemistry
- current research interests – inclusion complexes, non-covalent bonding, energetics of

Selected papers

1. Manakov A.Y., Lipkowski J., "The influence of the guest polarity on the clathrate structure formed by the Werner complex". *J. Incl. Phenom. Macro.*, **33**, 121 (1999).
2. Manakov A.Y., Lipkowski J., Pielaszek J., "Structure-properties relations in Werner beta-[Ni(NCS)(2)(4-MePy)(4)] clathrates. Part 2. Host-host interactions as a function of the guest molecular size and shape and the amount of absorbed guest compound". *J. Incl. Phenom. Macro.*, **35**, 531 (1999).
3. Manakov A.Yu., Soldatov D.V., Ripmeester J.A., Lipkowski J., "Zeolite like sorption of volatile organics in β-[CuL_2] (L={$CF_3COCHCOC(CH_3)_2OCH_3$}-)". *J. Phys. Chem. B*, **104**, 12111 (2000).
4. Weber E., Trepte J., Kravtsov V.Ch., Simonov Yu.A., "Ganin E.V., Lipkowski J., Heterocalixarene inclusion chemistry. Structure of a crystalline host-guest complex including endo-calix ethyl acetate and exo-calix clustering of water". *J. Incl. Phenom. and Macrocyclic Chem.*, **36**, 247 (2000).
5. Fonari M.S., Kravtsov V.Ch., Simonov Yu.A., Ganin E.V., Gelmboldt V.O., Lipkowski J., "Structure of the 18-Crown-6 Complex with Ammonium Hexafluorosilicate and Water". *J. Incl. Phenom. and Macrocyclic Chem.*, **39**, 85–89 (2001).
6. Branch C.S., Lewiński J., Justyniak I., Bott S.G., Lipkowski J., Barron A.R., "Aluminium and gallium compounds of salicylic and anthranilic acids: examples of weak-intramolecular hydrogen bonding". *J. Chem. Soc. Dalton Trans.*, 1253 (2001).
7. Samsonenko D.G., Lipkowski J., Gerasko O.A., Virovets A.V., Sokolov M.N., Fedin V.P., Platas J.G., Hernandez-Molina R., Mederos A., "Cucurbituril as a new macrocyclic ligand for complexation of lanthanide cations in aqueous solutions". *Eur. J. Inorg. Chem.*, 2380 (2002).
8. Kravtsov V.C., Fonari M.S., Zaworotko M.J., Lipkowski J., "A new polymorph of *cis*-transoid-*cis*-dicyclohexano-18-crown-6". *Acta. Crystallogr. C*, **58**, o683 (2002).
9. Lewiński J., Marciniak W., Ochal Z., Lipkowski J., Justyniak I., "A novel tetranuclear [MeZn(μ_3-OCH_2SMe)Zn(μ-Cl)Me]$_2$ adduct derived from interaction of CH_2Cl_2 with an alkylzinc complex". *Eur. J. Inorg. Chem.*, 2753 (2003).
10. Lewiński J., Ochal Z., Bojarski E., Tratkiewicz E., Justyniak I., Lipkowski J., "First structurally authenticated zinc alkylperoxide: a model system for the epoxidation of enones". *Angew. Chem. Int. Ed.*, **42**, (38), 4643 (2003).

Andrzej Bylicki, Professor Emeritus

M.Sc., 1951 – Department of Mathematics, Physics and Chemistry, Jagiellonian University, Cracow
Ph.D., 1957 – Department of Chemistry, University of Warsaw
Professor, 1965 – Institute of Physical Chemistry, Warsaw

Professional affiliations:

- Polish Chemical Society
- Polish Society of Calorimetry and Thermal Analysis
- Society for Advancement of Science and Arts (TPKN)
- International Council of Scientific Unions (ICSU) Committee on Data for Science and Technology (CODATA) Executive Committee member since 1980; Vice President 1984–1990 Task Group on Phase Equlibria, Chairmen 1982–1988, member 1988–1996

Editorial affiliations:

- John Wiley & Sons Ltd. Solubility Series Member of the Editorial Board

Research areas:

- Thermodynamics of solutions
- Experimental investigation and computation of phase equlibria and related thermodynamic properties in binary and multicomponent systems
- Cryomertic metods of investigation of solid-liquid equlibria in eutectic systems and solid solutions including extreme dilution range
- Methods of separation and purification of organic substances
- Investigation on solid-liquid-vapor equlibria in the systems forming associated solutions
- Liquid-liquid equlibria in systems containing electrolyte solution
- Physicochemical properties of coal chemicals
- Physicochemical properties and decarboxylation kinetics of pyridine-carboxylic acids

Selected papers

1. Bylicki A., "Kinetics of decarboxylation of pyridine-carboxylic acid", *Bull. Acad. Polon. Sci. Cl.III*, **6**, 633–638 (1958); *ibid*, **7**, 37–42 (1959).
2. Świętosławski W., Bylicki A. and Jankun J., "Mutual solubilities of pyridine bases in aqueous solution of electrolytes", *Bull. Acad. Polon. Sci. Ser. Chim.*, **1**, 7–10 (1961).
3. Bylicki A. and Bugajewski Z., "Studies on application of cryometry to the determination of purity in systems involving solid solution, in Thermal Analysis", vol. 2: "Organic and Macromolecular Chemistry", Akadémiai Kiadó, Budapest pp. 497–504 (1975).
4. Rogalski M. and Bylicki A., "Vapour pressures and excess Gibbs energies of {pyridine + (methyl- or ethyl- or *n*-propyl- or *n*-butylbenzene)} at T = 373.15 K", *J. Chem. Thermodyn.*, **17**, 915–919 (1985).
5. Gierycz P. and Bylicki A., "Correlation and Prediction of VLE ternary data by the NRTL equation", *Z. Phys. Chem.*, **269**, 731 (1988).
6. Bylicki A. and Gierycz P., "Prediction of phase equlibria in multiconponent mixtures", in "Scientific and Technical Data in a New Era" (P.S. Gleaser, Ed.), Hemisphere Publishing Corporation, New York pp. 151–157 (1990).
7. Plesnar Z. and Bylicki A., "Solid-liquid equlibria in alkohols + hydrocarbons systems", *International DATA Series, Selected Data on Mixtures*, **22**, 259–267 (1994).

Total number of publications: 112; patents: 16

Włodzimierz Kutner, Professor

M.Sc., 1971 – Chem. Dept., Warsaw University, Poland
Ph.D., 1975 – Chem. Dept., Warsaw University, Poland
D.Sc., 1995 – Institute of Physical Chemistry, Warsaw

Education and training:

1976–77 – Chem. Dept., University of Cincinnati, Cincinnati OH, USA (Postdoctoral Fellow)
1979 – J. Gutenberg University, Mainz, Germany (Visiting Scientist)
1983–84 and 1985 – Chem. Dept., University of North Carolina at Chapel Hill, Chapel Hill NC, USA (Research Associate)
1990–91 – Institute of Physical Chem. and Electrochemistry, Fritz-Haber-Institut der Max-Planck-Gesellschaft, Berlin, Germany (Visiting Scientist)
1991–93 – Chem. Dept., University of Houston, Houston TX, USA (Research Assistant Professor)
1994 – Institut für Festkörper- und Werkstofforschung, Dresden, Germany (Visiting Scientist)
1997, 1998, 1999, 2002 and 2003 – Chem. Dept., Wichita State University, Wichita KS, USA (Visiting Scientist)
2003 – Chem. Dept., University of Bordeaux 1, Bordeaux, France (Visiting Professor)

Professional affiliations:

- Polish Chem. Soc.; Active Member, 1975-onward; Vice President of the Warsaw Div., 1989–92.
- Electrochem. Soc., Fullerene Sect.; Active Member 1992–1994.
- IUPAC Commission on Electroanal. Chem. (V.5) of the Anal. Chem. Division; Affiliate Member, 1988–1990; Associate Member, 1990–1995; Titular Member, 1995–2001; Secretary of Commission V.5, 1998–2001; Associate Member of the Anal. Chem. Div. Committee, 2002–2005; Titular Member of the Interdivisional Committee on Terminology, Nomenclature and Symbols, 2002–2005.

Research areas:

- Supramolecular chemistry of inclusion polymers and moleculary imprinted polymers
- Electrochemistry and spectroscopy of fullerenes, carbon nanotubes and metalloporphyrins in the Langmuir and Langmuir-Blodgett films
- Electrodes modified with conducting polymers: electrochemical sensors and biosensors
- Simultaneous electrochemical and piezoelectric microgravimetry detection in flow analytical techniques
- Development of electroanalytical and piezoelectric microgravimetry instrumentation

Selected papers

1. Kutner W. and Galus Z., "Electrocatalytic oxidation of nickel amalgam in aqueous solutions of halogen and pseudohalogen ions", *J. Electroanal. Chem.*, **65**, 307–325 (1975).
2. Nowak R.J., Kutner W., Mark H.B. Jr. and MacDiarmid A.G., "Behavior of polymeric sulfur nitride, $(SN)_x$, electrodes in aqueous media", *J. Electrochem. Soc.*, **125**, 232–240 (1978).
3. Kutner W., Behr B. and Kemula W., "Detection of cholanoic acids in high-performance liquid chromatography based on effect of double layer capicity change at the dropping mercury electrode", *Fresenius Z. Anal. Chem.*, **312**, 12–1251 (1982).
4. Pickup P.G., Kutner W., Leidner C.R. and Murray R.W., "Redox conduction in single and bilayer films of redox polymer", *J. Am. Chem. Soc.*, **106**, 1991–1998 (1984).
5. Kutner W. and Doblhofer K., "Simultaneous cyclic voltammetry and electrochemical quartz-crystal microbalance study at the polymer film modified electrodes of molecular inclusion of ferrocene by the β-cyclo-dextrin polymer film and carboxymethylated β-cyclodextrin polymers as well as ferrocenecarboxylic acid by β-cyclodextrin polymer", *J. Electroanal. Chem.*, **326**, 139–160 (1992).
6. Koh W., Dubois D., Kutner W., Jones M.T. and Kadish K.M., "Electrosynthesis and electrodoping of C_{60}^{n-} (n = 0,1,2, or 3) films: electrochemical quartz crystal microbalance study in acetonitrile solutions of alkaline-earth-metal, or tetra(n-butylammonium cations", *J. Phys. Chem.*, **97**, 6871–6879 (1993).
7. D'Souza F., Choi J-p., Kutner W., "Catalytic reduction of α,ω-dihaloalkanes, $X(CH_2)_mX$ (X=Cl, Br or I and m=2 to 8), by electrochemically generated C_{70}^{n-} (n=2 to 3) in benzonitrile solutions", *J. Phys. Chem. B*, **102**, 4247–4252 (1998).
8. Marczak R., Hoang V.T., Noworyta K., Zandler M.E., Kutner W. and D'Souza F., "Molecular recognition of adenine, adenosine and ATP at the air-water interface by uracil appended fullerene", *J. Mater. Chem.*, **12**, 2123–2129 (2002).

Total number of publications: 106; patents: 5

Stanisław K. Malanowski, Professor Emeritus

M.Sc., 1953 – Department of Chemistry, University of Warsaw

Ph.D., 1960 – Institute of Physical Chemistry, Warsaw

D.Sc., 1974 – Institute of Physical Chemistry, Warsaw

Professor, 1987 – Institute of Physical Chemistry, Warsaw

Education and training:

1963–64 – Imperial College, London, Great Britain (visiting lecturer)

1979–80 – Technical University of Denmark, Lyngby (visiting professor)

1984–85 – University of Connecticut, Storrs, USA (visiting professor)

1993–94 – L'Ecole National Supérieure des Industries Chimiques de Nancy, France (professeur invité)

1996–97 – Universite de Metz, UFR Scientifiques, Institut de Physique et Chimie, Metz, France (professeur invité)

Professional affiliations:

- Polish Chemical Society
- American Chemical Society
- American Institute of Chemical Engineers
- ICSU Committee on Data for Science and Technology (CODATA) Task Group on Phase Equilibrium Data (1986–2001)
- International Union of Pure and Applied Chemistry (IUPAC) Committee on Thermodynamic Tables (1977–1987)

Editorial affiliations:

- Fluid Phase Equilibria, 1977–1995
- Thermodynamical Data for Technology, 1979–1988
- Chemical and Biochemical Engineering Quarterly, 1987 – present
- IUPAC – International Thermodynamic Tables of Fluid State, 1977–1987
- International Data Series – A. Selected Data on Mixtures, 1973–1985 & 1993–2001
- Journal of Chemical & Engineering Data, 2004–2006

Research areas:

- Measurements of vapour-liquid equilibria and other thermodynamic properties
- Methods for the representation of phase equilibria and fluid properties with emphasis on excess function models and the computation of phase equilibria and separation processes
- Thermodynamics of chemicals propagation in the environment

Selected papers

1. Malanowski S., "Vapour-liquid equilibrium, determination, calculation, application", PWN, Warszawa 1974 (in Polish).
2. Malanowski S. and Szafrański A. (Eds.), "Vapour-Liquid Equilibrium in Multicomponent Systems", PWN, Warszawa 1980.
3. Malanowski S., "Probleme der Modellierung von Mehrstoffsystemen, chapter in „Modellierung von Phasengleichgewichten als Grundlagen Stofftrennprozessen", Akademie-Verlag, Berlin 1981, pp. 328–372.
4. Stephenson R.M. and Malanowski S., Handbook of the Thermodynamics of Organic Compounds", Elsevier, New York 1987.
5. Malanowski S. and Anderko A. (Eds.), "Thermodynamics of Fluids: Measurement and Correlation", First Edition, Institute of Physical Chemistry, Warsaw 1989, pp. 499; Second Edition, World Scientific Publishing Co., Singapore 1990, pp. 514.
6. Malanowski S. and Anderko A., "Modelling Phase Equilibria: Thermodynamic Background and Practical Tools", J. Wiley, New York 1992, pp. 311.

Total number of publications: *ca.* 200

Joanna Taraszewska, Professor

M.Sc., 1959 – Department of Chemistry, University of Warsaw
Ph.D., 1967 – Institute of Physical Chemistry, Warsaw
D.Sc., 1987 – Institute of Physical Chemistry, Warsaw
Prof. – 1997

Education and training:

1969 – Max Planck Institute of Physical Chemistry, Göttingen, Germany (Postdoctoral Research Fellow)
1979–80 – Colorado State University, Fort Collins, USA (Research Associate)
1983 – University of Milan, Italy (Research Assistant Professor)
1993–1995 – University of Pavia, Italy (Research Associate Professor)

Professional affiliations:

- Polish Chemical Society (since 1959, Secretary of the Main Goverment 1970–1974, Chairman of the Main Revision Commission 1975–1979)
- International Union of Pure and Applied Chemistry (IUPAC)
- International Society of Electrochemistry (ISE)

Research areas:

Characterization of physicochemical properties, and particulary of the redox behaviour of supramolecular complexes containing transition metal ions

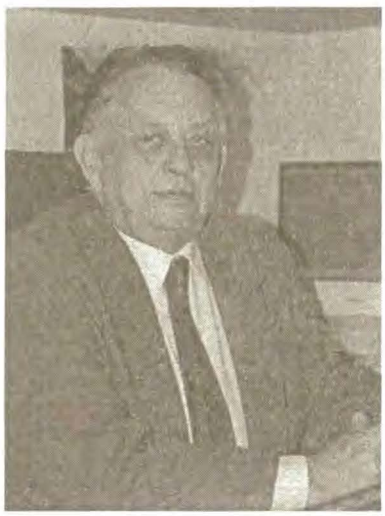
- Modification of electrodes with macrocyclic complexes-application in electrocatalysis
- Study of polynuclear azamacrocyclic complexes
- Azamacrocyclic transition metal complexes with appended crown ethers as electrochemical sensors
- Study of cyclodextrin inclusion complexes directed on pharmaceutical applications

Selected papers

1. Taraszewska J., Rosłonek G. and Darlewski W., "Electrochemical behaviour of nickel tetraazamacrocyclic complexes incorporated into carbon paste electrodes: application in H_2O_2 electrocatalysis", *J. Electroanal. Chem.*, **371**, 223–230 (1994).
2. Bukowska J., Rosłonek G. and Taraszewska J., "In-situ surface- enhanced Raman spectroscopic study of gold electrodes modified with nickel tetraazamacrocyclic complexes", *J. Electroanal. Chem.*, **403**, 47–52 (1996).
3. Taraszewska J., Rosłonek G., Lampeka Ya.D. and Maloshtan I.M., "Oxalate-bridged dinuclear nickel azacyclam macrocyclic complexes: synthesis and electrochemical study", *J. Electroanal. Chem.*, **452**, 49–56 (1998).
4. Taraszewska J., Rosłonek G. and Korybut-Daszkiewicz B., "Redox properties of novel dinuclear Ni(II) bis-tetraazamacrocyclic complex", *Supramolecular Chem.*, **12**, 115–121 (2000).
5. Taraszewska J., Migut K. and Kożbiał M., "Complexation of flutamide by native and modified cyclodextrins", *J. Phys. Org. Chem.*, **16**, 121–126 (2003).
6. Taraszewska J., Zięba K., Korybut-Daszkiewicz B., "Crown ethers appended copper tetraazamacrocyclic complexes as receptors for cationic guests", *Electrochim. Acta*, **49**, 2675–2681 (2004).

Total number of publications: 70

Wojciech Zielenkiewicz, Professor Emeritus



M.Sc., 1955 – Department of Mat.-Fiz.-Chemistry, University of Warsaw
Ph.D., 1961 – Institute of Physical Chemistry, Warsaw
Professor, 1971 – Institute of Physical Chemistry, Warsaw
Titular Professor, 1987 – Institute of Physical Chemistry, Warsaw

Professional affiliations:

- Foreign Member of the Royal Academy of Sciences, Barcelona, Spain (since 1975)
- Corr. Member of the Polish Academy of Sciences (since 1977)
- IUPAC Associate and Titular Member 1.2. Commission of Thermodynamics (1977–1987). Affiliate Member (since 1988)
- Polish Chemical Society
- Polish Physical Society
- Polish Society of Calorimetry and Thermal Analysis, W. Swietoslawski – President and then Honorary President
- American Chemical Society
- International Society Nucleosides, Nucleotides and Nucleic Acids

Research areas:

Thermodynamics, thermochemistry and calorimetry:

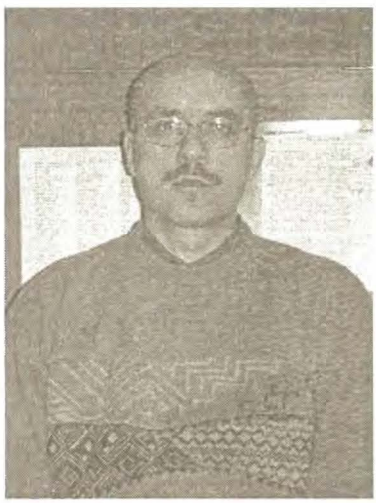
- The theory of calorimetry
- Selected problems of biothermodynamics: thermodynamics investigations of enzymes and proteins, solutions of nucleic acid bases, conformational changes of nucleic acid and proteins
- Thermodynamics of inclusion compounds. Determination of constants binding, changes of free Gibbs energy, enthalpy and entropy, partial molar volumes and heat capacities
- Heat of combustion using the fluorine calorimetric bomb and oxygen rotating calorimetric bomb.

Selected papers

1. Zielenkiewicz W., Margas E., "Fundamentals of dynamic calorimetry" Ossolineum, Wrocław, pp. 152 (in Polish). Russian edition: "Teoreticheskiye osnovy dinamicheskoy kalorimetrii", Tipografiya GUKPK Mintopenergo RF, Ivanovo, Russia 1993 (pp. 191).
2. Zielenkiewicz W., Hatt J., Margas E., Torra V., Berger R.L., Mudd C.P. and Schuette W., "Thermokinetics. Signal Processing in Calorimetric System". Editor: Zielenkiewicz W., Ossolineum, Wrocław, 1990 (pp. 274).
3. Zielenkiewicz W., Margas E., "Theory of Calorimetry", Kluwer Academic Publishers B.V., Dordrecht/Boston/London, 2002 (str.. 215).
4. Georgalis Y., Umbach P., Zielenkiewicz A., Utzig E., Zielenkiewicz W., Zielenkiewicz P. and Saenger W., "Microcalorimetric and small-angle light scattering studies on nucleating lysozyme solutions", *J. Am. Chem. Soc.*, **119**, 11959–11965 (1997).
5. Zielenkiewicz W., "Determination of Heat Effects. Method and Applications.", (in Polish), Polish Academy of Sciences, CUNPAN, Warsaw, 2000, (pp. 177).
6. Komorowski S.J., Grabowski Z.R. and Zielenkiewicz W., "Pulsed photoacoustic determination of quantum yield of triplet state formation", *J. Photochem.*, **30(2)**, 141–151 (1985).
7. Zielenkiewicz W., "Aqueous solutions of pyrimidine nucleic acid bases. Solute-solvent interactions", *Pure App. Chem.*, **71(7)**, 1285–1290 (1999).
8. Kuliński T., Bratek-Wiewiórowska M.D., Wiewiórowski M., Zielenkiewicz A., Żółkiewski M. and Zielenkiewicz W., "Comperative calorimetric studies on the dynamic conformation of plant 5SrRNA", *Nucl. Acids Res.*, **19**, 2449–2455 (1991); *ibid*, **16**, 685–701 (1988).
9. Zielenkiewicz W., "Thermodynamic investigations on derivatives of pyrimidine nucleic acid bases. Joint use of calorimetric, volumetric and structural data for the description of properties of pyrimidine nucleic acid bases their derivatives", *Thermochim. Acta*, **405**, 1–15 (2003).

Total number of publications: 213

Jacek Gregorowicz, Associate Professor



M.Sc., 1980 – Department of Chemistry, Warsaw University of Technology
M.Sc., 1987 – Faculty of Mathematics, Informatics and Mechanics, University of Warsaw
Ph.D., 1990 – Institute of Physical Chemistry, Warsaw
D.Sc., 2001– Institute of Physical Chemistry, Warsaw

Education and training:

1989–1990 – University of Trieste, Italy
1991–1994 – Delft University of Technology, The Netherlands

Research area:

- High pressure phase equilibria
- Thermodynamics of phase equilibria
- Application of supercritical fluids to polymer processing

Selected papers

1. Gregorowicz J., Fermeglia M., Soave G. and Kikic I., "The Perturbed -Hard – Chain theory for the prediction of supercritical fluid extraction: Pure compounds properties", *Chem. Eng. Sci.*, **46**, 1427–1436 (1991).
2. Chyliński K. and Gregorowicz J., "Liquid phase PVT – data of alkylbenzenes", *Fluid Phase Equilibria*, **64**, 237–249 (1991).
3. Gregorowicz J., de Loos Th.W. and de Swaan Arons J., "Unusual retrograde condensation in ternary hydrocarbon systems", *Fluid Phase Equilibria*, **73**, 109–115 (1992).
4. Gregorowicz J., de Loos Th.W. and de Swaan Arons J., "Three phase equilibria in the binary system ethylene + eicosane and the ternary system propane + ethylene + eicoasne", *J. Chem. Eng. Data*, **38**, 417–421 (1993).
5. Gregorowicz J., "Solubilities of lactic acid and 2-hydroxyhexanoic acid in supercritical carbon dioxide", *Fluid Phase Equilibria*, **166**, 39–46 (1999).
6. Gregorowicz J. and de Loos Th.W., "High pressure phase equilibria in asymmetric binary and ternary hydrocarbon mixtures", *Ins. Eng. Chem. Res.*, 40, 444–451 (2001).

Total number of publications: 30

Stanisław Randzio, Associate Professor

M.Sc., 1965 – Department of Chemistry, University of Warsaw, Warsaw

Ph.D., 1975 – Institute of Physical Chemistry, Warsaw

D.Sc., 1985 – Institute of Physical Chemistry, Warsaw

Education and training:

1966–67 – Graduate Student, Centre de Recherche de Micracalorimétrie et de Thermochimiche CNRS, Marseille, France,

1976–77 – Post-doctoral Research Fellow University of Lund, Sweden

1985–86 – Senior Research Fellow, Brigham Young University, Provo, USA

1991 – Visiting Professor, Brigham Young University, Provo, USA

1993 – Senior Research Fellow, Blaise Pascal University, Clermont-Ferrand, France

1996–1999 (four months each year) – Invited Professor, Blaise Pascal University, Clermont-Ferrand, France 2001, 2003 – Invited Professor, University of Paris XI, France

Professional affiliations:

International Union of Pure and Applied Chemistry (IUPAC), Commission on Thermodynamics (I.2) of the Physical Chemistry Division (I), Associate Member (1987–1995)

Editorial affiliations:

Member of the Editorial Board of Thermochimica Acta (1996–2003)

Research areas:

Thermophysics and transitiometry of condensed matter and interfaces:

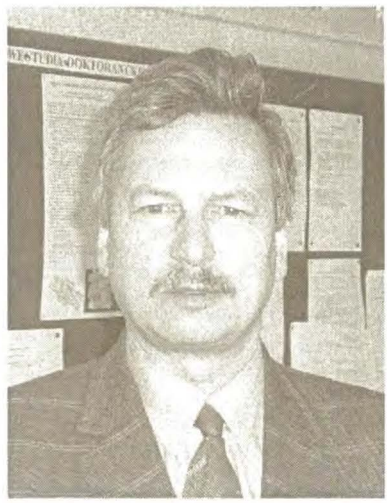
- micro- and nano-structured materials;
- phase transitions in macromolecular and asymmetric systems;
- polymers under near-critical conditions;
- polymorphism;
- piezothermal properties of liquids and fluids.
- transitiometry, including at supercritical conditions

Selected papers

1. Randzio S.L. and Suurkuusk J., "Interpretation of calorimetric thermograms and their dynamic corrections", chapter in "Biological Microcalorimetry" (A. Beezer, Ed.), Academic Press, 1980, pp. 311–341.
2. Randzio S.L., "Calorimetric determination of pressure effects on the thermodynamic properties of liquids", chapter in "Experimental Thermodynamics, vol. 4: Solution Calorimetry" (Eds. P.A.G. O'Hare and K.N. Marsh), Blackwell Scientific 1994, pp. 303–324.
3. Randzio S.L., "From calorimetry to equations of state", *Chem. Soc. Rev.*, **24**, 359–366 (1995).
4. Randzio S.L., "Scanning Transitiometry", *Chem. Soc. Rev.*, **25**, 383–392 (1996).
5. Randzio S.L. and Grolier J.P-.E."Supercritical Transitiometry of polymers", *Anal. Chem.*, **70**, 2327–2333 (1998).
6. Randzio S.L., "Recent developments in calorimetry", *Ann. Rep. Prog. Chem., (The Royal Society of Chemistry)*, Sect. C, **94**, 433–504 (1998).
7. Randzio S.L., Flis-Kabulska I. and Grolier J.-P.E., "Reexamination of phase transitions in the starch-water system" *Macromolecules*, **35**, 8852–8859 (2002).
8. Randzio S.L., "Recent developments in calorimetry", *Ann. Rep. Prog. Chem. (Royal Soc. Chem.), Sect. C*, **98**, 157–217 (2002).
9. Randzio S.L., Flis-Kabulska I. and Grolier J.-P.E., "Influence of fiber on the phase transformations in the starch-water system", *Biomacromolecules*, **4**, 937–943, (2003).

Total number of papers: 85

Paweł Gierycz, Research Associate



M.Sc., 1977 – Institute of Chemical Engineering, Technical University of Warsaw
Ph.D., 1982 – Institute of Physical Chemistry, Warsaw
D.Sc., 2001 – Faculty of Process and Environmental Engineering, Technical University of Łódź

Education and training:

- 1978 – Institute of Theoretical Fundamentals of Chemical Technology of the CSAS, Prague, Czechoslovakia
- 1985 – Marseilles University, Marseilles, France
- 1983–1984 – Kyoto University, Kyoto, Japan
- 1990 – Erlangen University, Erlangen, Germany
- 1990–1991 – Kanazawa University, Kanazawa, Japan

Professional affiliations:

- Chief Technical Organisation (NOT)
- Polish Society of Calorimetry and Thermal Analysis
- Director of the Centre of Excellence: Thermodynamic Laboratory for Environmental Purposes

Research areas:

- Thermodynamics of phase equilibria
- Calorimetry
- Supercritical Extraction
- Nanomaterials

Selected papers

1. Gierycz P., "Computer simulation – application to thermodynamic models." a chapter in the book: "Thermodynamics for Environment", edited by Gierycz P. and Malanowski S., Information Processing Centre, Warszawa, 73 (2004).
2. Gierycz P., "Mathematical Modeling of Vapour-Liquid Equilibria." a chapter in the book: "Thermodynamics for Environment", edited by Gierycz P. and Zielenkiewicz W., Information Processing Centre, Warszawa, 355 (2003).
3. Gierycz P. , "Methods of Correlation and Prediction of Vapour-Liquid Equilibria of Multicomponent Systems." a chapter in the book: "Thermodynamics for Environment", edited by Gierycz P. and Zielenkiewicz W., Information Processing Centre, Warszawa, 373 (2003).
4. Gierycz P., "New local composition model for excess Gibbs energy. III. Extension for coassociation and multicomponent mixtures." *Polish J. Chem.*, **70**, 1193 (1996).
5. Gierycz P., "Comparison and verification of methods for correlation and prediction of VLE in multicomponent systems." *Polish J. Chem.*, **70**, 1373 (1996).

Total number of publications: 57

Laboratory of Calorimetry

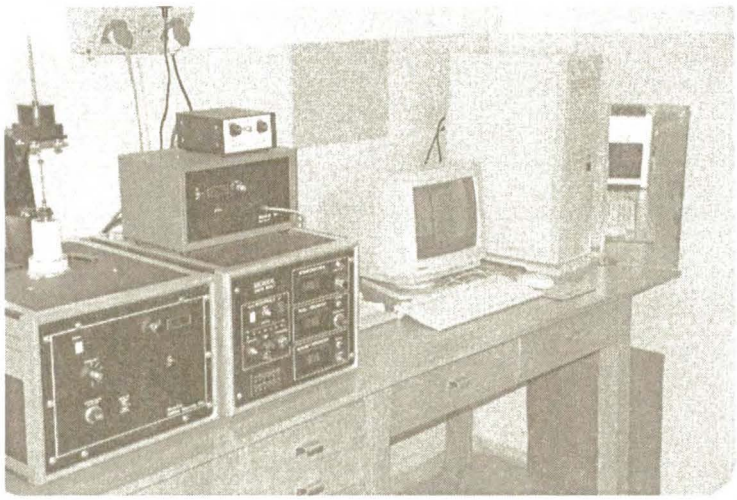
Head: Prof. Wojciech Zielenkiewicz

Thermodynamic properties of organic compounds

We offers possibilities to determine the enthalpy of combustion, the enthalpy of solution, enthalpy of dilution and mixing, heat of chemical reaction, partial molar volumes and heat capacities, thermokinetics of reaction, vapour pressure of solid compound, the enthalpy of sublimation and thermoanalytical determination, *e.g.* specific heat of solid compounds, temperature and the enthalpy of fusion, determination of thermodynamic parameters under high pressure.

Equipment

- Isothermal titration calorimeter for determination of binding constants (K), reaction stoichiometry (n), enthalpy (H) and entropy (S) of reaction of complexation (Microcal OMEGA). Specifications: total volume of vessel: 1.3 ml; temperature range: 2 ÷ 80°C; sensitivity: 0.1 μcal·s^{-1}.
- Isoperibol solution calorimeter. Specifications: volume of reaction vessel 150 cm^3; range of temperature 20÷50°C; accuracy of temperature determination 2·10^{-3}oC; sensitivity 5·10^{-2} cal·min^{-1}, the mass of the substance used 10–30 mg.
- Microcalorimetr LKB 10700 batch, flow, adsorption for determination of the enthalpy of mixing and dilution. Specifications: range of temperature 20÷40°C, stability 0.001°C, sensitivity: 0.5 μW, accuracy: 1%.
- Conduction calorimeter for measuring the total heat effects and thermokinetics. Specifications: volume of the calorimetric cell: 30 cm^3; mass of the sample: 10÷20 g; temperature range: 20÷50°C; time constant: 780 s; heat loss coefficient: 7.7 W·V^{-1}.
- Thermal analysis devices: Du Pont Thermal Analyst System 2100; Calvet TG-DSC 111 SETARAM. Specifications (Calvet TG-DSC 111 SETARAM): mass of substance: 0.5÷100 mg; range of temperature: –180 ÷ 800°C. Specifications of Du Pont Thermal Analyst System 2100: mass of the substance 0.5 ÷ 100 mg; sensitivity (DTA, TGA) 0.4%, (DSC) 1%; range of the temperature (DSC) 180°C ÷ 700°C; (DTA) 180°C ÷ 700°C; (TGA) 20°C÷1200°C.
- Heat conduction microcalorimeter for thermokinetics investigations, titration experiments, heat effect of reaction. Specifications: sensitivity: 103 μV·mW^{-1}; total volume of vessel: 3 cm^3 ; time constant: 151 s; lowest detectable continuous heat effects: 6·10^{-7}W.
- The measurement of vapour pressure and the enthalpy of sublimation with use of two methods: inert gas flow method and Knudsen method. Specifications (inert gas flow method): temperature range: to 300°C; sample capacity: about 30 mg. Specifications of Knudsen method: temperature range: 20 ÷ 270°C; sample capacity: above 100 mg; sensitivity: 0.5 ÷ 4%.
- Density measurement used to determination of the apparent volume changes (Densimeter DMA60/602, Anton PAAR). Specifications: accuracy: ±1.5·10^{-6} g·cm^{-3}; temperature coefficient: –3·10^{-4} g·cm^{-3}·K^{-1}; pressure coefficient: –5·10^{-5} g ·cm^{-3} ·bar^{-1}; sample size: 0.7 cm^3; sensitivity: 1 g·cm^{-1}.



- Microcalorimeter DASM-4 to observation changes of heat capacities and heat of conformational changes of biopolimers. Specifications: volume of the cell: 0.5 ml; temperature range: 250÷400 K; heating rates: 0.1÷2 $K \cdot min^{-1}$; sensitivity: 0.2 μW; accuracy: 0.05 $mJ \cdot K^{-1}$.

Contact persons:

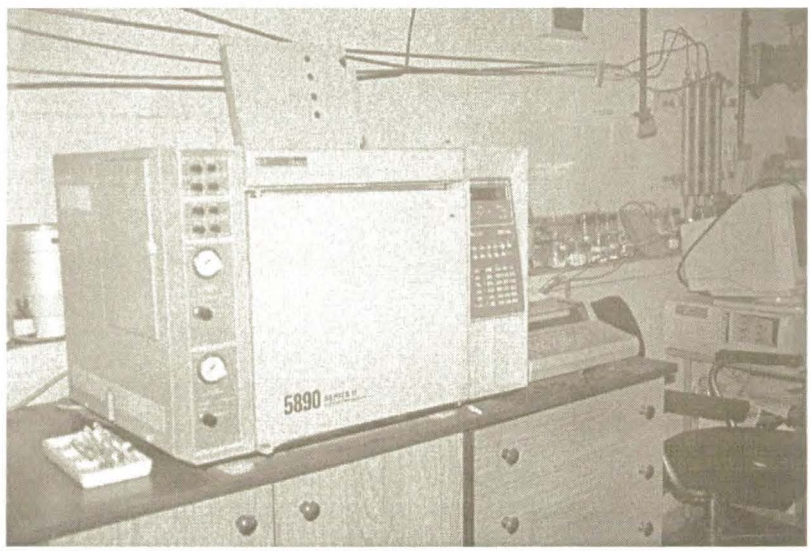
Prof. Wojciech Zielenkiewicz, e-mail: zivf@ichf.edu.pl

Dr. Małgorzata Wszelaka-Rylik, e-mail: malg@ichf.edu.pl

Laboratory of Chromatographical Analysis

Head: Dr. Anna Bielejewska

Phone: +48 (22) 343-3415
e-mail: annab@ichf.edu.pl
Build. 7, room 244b



Expert Laboratory of Chiral Chromatography performs chromatographic studies of mixtures which are otherwise separable with difficulty, *e.g.*

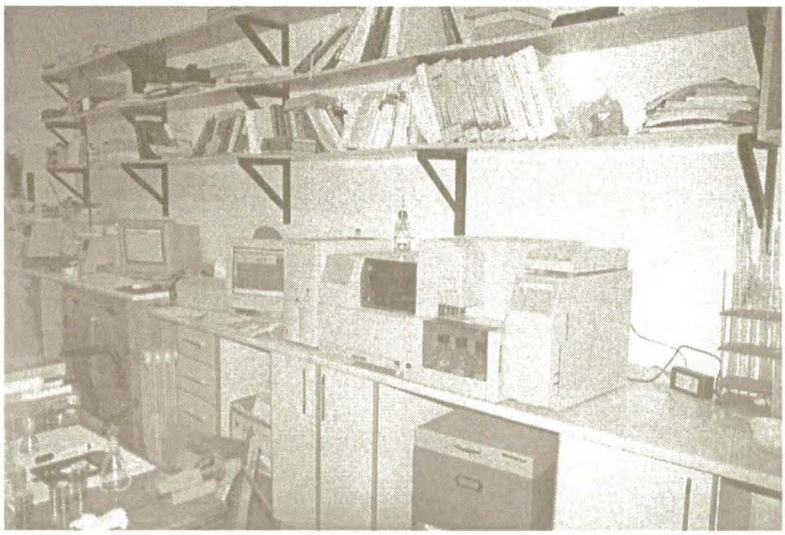
- enantiomeric composition of terpenic hydrocarbons in essential oils (it has been found that quality and quantity of terpens produced by plants depends not only from genetic fac-tors but also from micro and macro environment)
- enantiomeric composition of some therapeutics applied in the treatment of liver and kid-ney diseases (they differ from one another by enantiomeric composition)
- micro preparative methods for ultra pure standards of optically active hydrocarbons (*e.g.* (-) camphene samples of 94% enantiomeric purity)
- methods to control enantiomeric purity of chiral drugs (*e.g.* bromofosfamide and its me-tabolites).

The area of research includes physicochemical studies on complexation processes themselves (stability, stoichiometry, thermodynamic functions)

Our equipment includes:

Gas chromatography:

Two Hewlett-Packard Model 5890 gas chromatographs with FID detectors. Chiral capillary columns modified by various derivatives of cyclodextrins. Classical columns covered with solutions of cyclo-dextrins.



Liquid chromatography:

Waters and Knauer chromatographs equipped with RI, Chiralyser and UV-VIS detectors. As the chiral selectors we use native cyclodextrins, cholic acids and its derivatives as the additives to the mobile phase.
We also have chiral columns: *e.g.* Cyclobond I 2000, Chiracel OD and Chiralpak AD

Capillary Elektrophoresis:
Thermo Separation CE Ultra apparatus.

Contact persons:

Dr. Anna Bielejewska, e-mail: annab@ichf.edu.pl
Dr. Monika Asztemborska, e-mail: monika@ichf.edu.pl
The details can be obtained:
Department II. Institute of Physical Chemistry PAS
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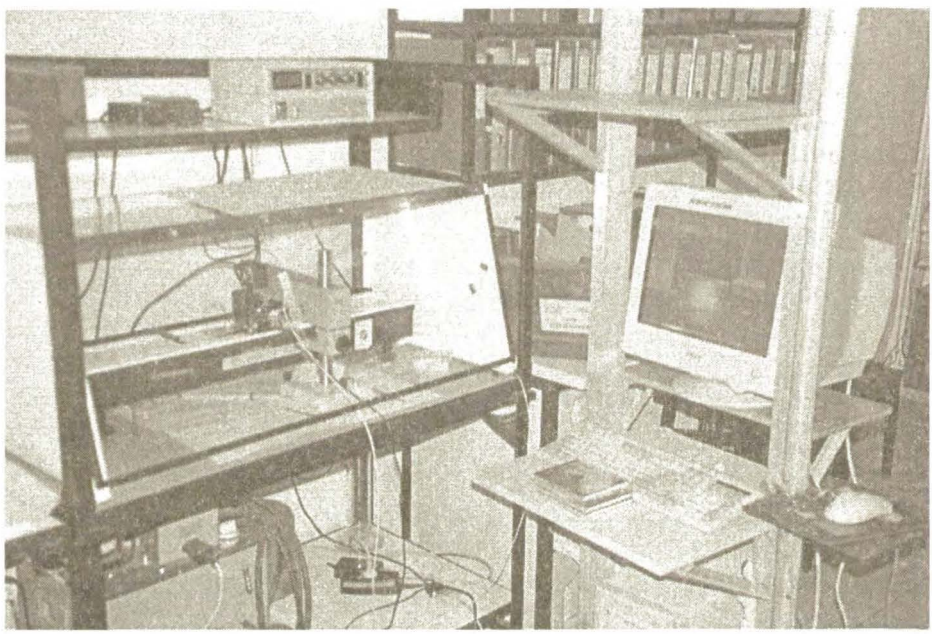
Laboratory of Molecular Films

Head: Prof. Włodzimierz Kutner

Phone: +48 (22) 343-3217
Fax: +48 (22) 632-5276
E-mail: wkutner@ichf.edu.pl



Purity of samples used for film preparation is examined with a gradient HPLC system composed of two pumps Model 6000 of Waters, Millipore Corp. (Milford MA, USA) and a home made gradient controller as well as a UV-vis detector type SPD10A of Shimadzu Corp. (Tokyo, Japan) or a home made electrochemical detector. These samples are purified, if needed, by using a semi-preparative mode of this HPLC system.

Mono- and multilayer Langmuir films floating on aqueous subphase solutions are prepared and their spreading properties investigated by using a rectangular trough, type BAM 601 of Nima Technology, Ltd., (Coventry, UK). During the film compression and expansion, surface pressure and surface potential are simultaneously measured with a Nima PS-4 surface pressure (Wilhelmi plate) sensor and a Nima KP-2 surface potential (Kelvin probe) sensor, respectively. Moreover, the film morphology is imaged continuously during compression-expansion cycling with a Brewster angle microscope type MiniBAM of NFT-Nanofilm Technologie, GmbH (Göttingen, Germany).

With a Nima D1L linear dipper, the Langmuir films are vertically transferred, by using the Langmuir-Blodgett (LB) technique, onto solid substrates, such as quartz slides, indium-tin oxide (ITO) slides or highly oriented pyrolytic graphite (HOPG) specimens, or onto quartz crystal oscillators for UV-vis spectroscopy, UV-vis spectro-electrochemistry or simultaneous electrochemical and piezoelectric microgravimetrical characterization, respectively. Moreover, the monolayer films are prepared on solid substrates by self-assembly while multilayer films by electrochemical polymerization, dip- or spin-coating as well as electrochemical polymerization, or either electrophoretic or vacuum deposition.

With a Monolayer/Grazing Angle Accessory for FT-IR Spectroscopy of Graseby Specac, Ltd. (Kent, UK) the IR spectra are recorded with a 170SX FT-IR spectrometer of Nicolet (Madison, WI, USA) of either floating Langmuir films or those transferred onto solid substrates by using the LB technique.

For simultaneous piezoelectric microgravimetry and electrochemistry measurements electrochemical quartz crystal microbalances of the Institute of Physical Chemistry (Warsaw, Poland) are used. The 5 or 10 MHz quartz crystal oscillators serve for operation under steady-state (Model EQCM 5510 and 5710) or flow-through (EQCM 5610) solution conditions. The EQCM 5610 microbalance features a flow-through quartz crystal holder suitable for simultaneous piezoelectric microgravimetry and electrochemical detection measurements in flow analytical techniques, such as flow injection analysis (FIA) and micro-bore column HPLC. The EQCM 5710 microbalance is used for simultaneous measurement of current or charge, frequency or frequency changes and dynamic resistance allowing thus for measurement of both mass and viscoelastic changes during an electrochemical process.

Viscoelastic properties in solutions of films and mass changes are also simultaneously examined by analyzing components of electromechanical impedance of the film-coated quartz crystal oscillators in air and in solution. For that purpose, an 8712E RF Network Analyzer of Agilent Technologies (Englewood, CO, USA) is used, along with a dedicated VEE software, either in a transmission (in air) or reflection (in air and in solution) mode of operation. Analysis of the viscoelestic film properties can be performed under electrochemical conditions if the Autolab electrochemistry system (see below) is connected.

Electrochemical measurements on films are carried out with a driven by dedicated GPES 4.5 software two Autolab electrochemical systems of Eco Chemie (Utrecht, The Netherlands), equipped with cards of a PGSTAT20 potentiostat, BIPOT bipotentiostat, ECD microelectrode unit, and FRA frequency response analyzer, which is used for measurements of the electrochemical impedance spectroscopy. Moreover, rotating ring-disk electrode (RRDE) voltammetric and chronoamoperometric measurements on the films are performed.

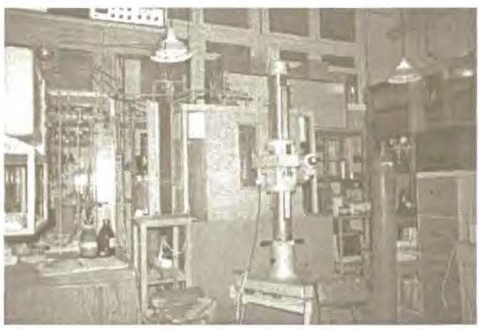
Contact persons:

Prof. Włodzimierz Kutner; wkutner@ichf.edu.pl
Renata Marczak, M.Sc.; rmarczak@ichf.edu.pl
Agnieszka Kochman, M.Sc.; agakoch@ichf.edu.pl
Piotr Pięta, M.Sc.; ppieta@ichf.edu.pl
Agnieszka Pietrzyk, M.Sc.; agapi@ichf.edu.pl

Laboratory of Thermodynamics

Head: Prof. Stanisław K. Malanowski

Tel.: 48 (22) 632 67 13
e-mail: skm@ichf.edu.pl



The Laboratory of Thermodynamics is devoted to measurements and computation of thermodynamic properties of pure organic compounds and mixtures of these. The main interest is focused on the development of theoretical and empirical methods for the measurement, prediction and correlation of phase equilibrium and related thermodynamic properties. The necessary equipment is constructed and assembled in the Laboratory.

Our service focuses on most important information for process design. Our experimental facilities comprise a variety of equipment for the determination of pure component properties (vapor pressures, liquid densities, etc.), phase equilibrium (VLE, azeotropic data, activity coefficients at infinite dilution, LLE, SLE, gas solubility, Henry coefficients, *etc.*) and excess volumes. The choice between static or dynamic, synthetic or analytic, batch and flow apparatus allows to apply the most suitable technique for a given problem (pressure and temperature range, nature of the compounds and their mixtures). The measurements are made in a pressure range up to 8 MPa and a temperature range between 70 and 400 K. We provide our customers with the most reliable data in a short time, depending on the extent of the demand.

The Laboratory has permanent contracts with American Institute of Chemical Engineers (DIPPR Project 805).

In recent years laboratory has delivered equipment for determination of phase equilibrium to following customers:

- Dipartamento di Energetica, Universita di Ancona 60100 Ancona, Italia
- Enichem Spa, *via* G. Fauser 4, 28100 Novara, Italia
- OIKOlab, Marathonos Str. 63, Gerakas, 153 44 Athens, Greece
- Istituto per la Tecnica del Freddo - cnr, Corso Stati Uniti, 4, 35127 padova, Italia
- Université de Metz, Laboratoire de Thermodynamique et d'Analyse Chimique, Ile du Saulcy, F-57045 Metz, France
- Department of Chemical Engineering, University of Delaware, 114 Colburn Laboratory, Newark, DE 19716 USA.
- Department of Chemical Engineering, Mississippi State University 129 Etheredge Building, MS 39762 USA.

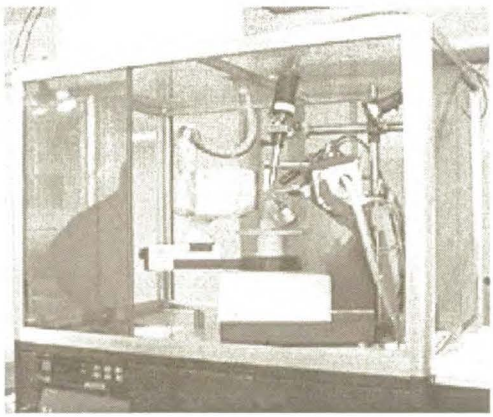
Contact person:

Prof. Stanisław K. Malanowski,
E-mail: skm@ichf.edu.pl
Phone: +(48 22) 343-3246

Laboratory of X-Ray Structural Analysis

Head: Prof. Janusz Lipkowski

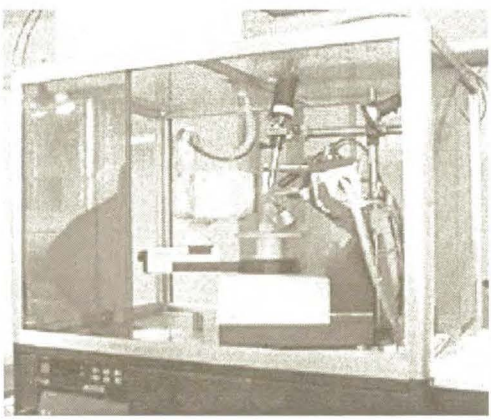
Tel.: (0 22) 343-3213 or 343-3254,
room 234, 245
e-mail: klatrat@ichf.edu.pl



Laboratory of X-Ray Structural Analysis, being a part of the Department II, is specialized in investigation of crystal and molecular structures by X-ray diffraction on single crystals and powder specimens. Equipped with two automatic diffractometers for single crystals Nonius KappaCCD and KUMA Diffraction KM-4, and one powder diffractometer Bruker AXS D8 Advance, is prepared to perform a complete structural analysis from data collection through data reduction, structure solution, structure refinement to graphical representation of the structure. Scientific staff working in the Laboratory is experienced in crystallography of organic, inorganic and organometallic compounds. Additionally, it is also possible to perform analysis of phase composition and texture study of powder samples. Diffraction measurtements can be performed at controlled temperature within the range from 80 to 400 K using LT device of OXFORD CRYOSYSTEMS Series 700.

Scientific projects actually performed within Laboratory include:

1. Physicochemistry and structural chemistry of supramolecular complexes including chiral systems.
2. Structure and dynamics of supramolecular complexes.
3. Analysis of phase composition.
4. Data collections and structural analysis for other scientific groups.



More information:

Dr. Kinga Suwińska, kinga@ichf.edu.pl
Dr. Iwona Justyniak, iwona@ichf.edu.pl

III. Department of Soft Condensed Matter and Fluids

Head: Professor Robert Hołyst

There are two main research topics in the Department III

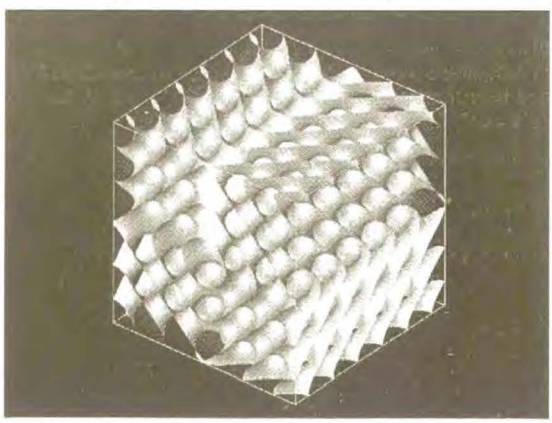
1. Study of phase transitions (including kinetics of these transitions) and the structure of liquid crystals, polymers, microemulsions and ionic liquids.
2. Surface phenomena in soft matter including adsorption, structure of interfaces, structure of systems in restricted geometry.

At the beginning of 1970s Professor Stecki began to develop statistical thermodynamics of liquid crystals in the Department and also the density functional theory to phase transitions, structures and elastic properties of liquid crystal systems. The result of this research in liquid crystal systems was the discovery of a close relation between nematic elastic constants and correlation functions. The density functional theory was also generalised to include highly correlated (dense) liquid crystal systems in the form of the weighted density approximation.

Since 1990 the Department has begun research on polymer solutions, polymer mixtures, surfactant mixtures and mixtures of polymers and surfactants apart from the study of liquid crystals. The most important achievement in this research was the discovery of complicated structures created by mixtures of water, surfactants and carbohydrates (1996). The discovery included a gyroid structure of genus 157, which is the most complicated structure known in the world so far. It gave rise to the use of geometry and topology in the study of kinetics and dynamics of phase transitions. Since 2000, along with the theoretical research, experimental works have been carried out in the Department, including experiments using laser light scattering, optical microscope, electrophoresis as well as small angle X-ray scattering applied for soft matter structures (gels, mixtures of polymers, liquid crystals, surfactants).

At present new topics are studied including protein diffusion between membranes in surfactant mixtures with water; dynamic light scattering on micelles in surfactant mixtures with water and dewetting in liquid helium.

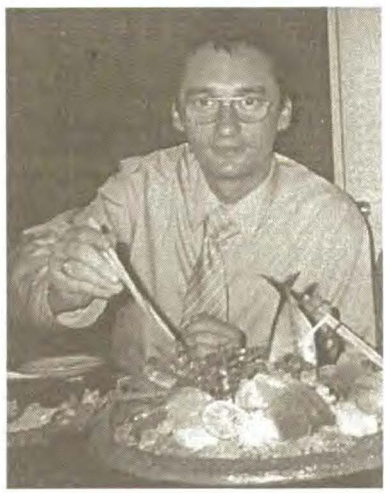
The staff of the Department III cooperates with scientists from many centres in the world: in USA (Harvard, University of Minnesota, University of Washington, Oregon State University, University of Chicago, University of Illinois Urbana-Champaign, Northwestern University, Stony Brook University), France (Ecole Normale Superieure), Germany (Max Planck Institutes in Stuttgart, Mainz and Teltow, University of Paderborn, Technical University of Berlin, University in Essen), Japan (Mitsui Chemicals Inc.), South Korea (Samsung Advanced Institute of Technology), England (Oxford, Bristol University, University in Southampton), Norway (Trondheim University) and Belgium (University of Brussels).



www.ichf.edu.pl/Dep3.html

In the years 1995-1997 a theoretical method for creating periodic surfaces of unrestricted complexity was discovered in the Department III. Scientists in the world had worked on this problem since the end of 19th century. The picture shows the structure of genus (number of holes) 157 obtained by means of this method and so far it has been the most complex periodic structure known in the world. Such structures existing in nature (block copolymers, surfactants or zeolites) awake interest in mathematicians, chemists and physicists and are applied as mesoscopic sieves, catalyzers, high resistance light materials, photonic crystals or materials for holography). Our works have aroused interest in chemists from the Imperial College and Cambridge (Prof. J. Kalinowski, a most frequently quoted Polish chemist) and physicists from Princetown University as well as a mathematician, Alan Schoen, who in 1970 made the most significant discoveries in the field of periodic surfaces since the end of 19^{th} century.

Robert Hołyst, Professor



M.Sc., 1986 – Department of Physics, University of Warsaw
Ph.D., 1989 – Institute of Physical Chemistry, Warsaw
D.Sc., 1992 – Institute of Physical Chemistry, Warsaw
Professor 1998 – Institute of Physical Chemistry, Warsaw

Education and training:

1989–1991 – Postdoctoral Research Associate, University of Washington, USA
1993, 1994, 1995 (4 months). Visiting Fellow, Max Planck Institute for Polymer Science, Mainz, Germany
1995, 1997 (8 months). Visiting Scientist, Ecole Normale Superiere, Lyon, France
1998, 2000–2002 (16 months). Visiting Professor, Ecole Normale Superiere, Lyon, France
1994–1996 Vice-Rector College of Science, Warsaw, Poland
2001 – Head of Department, Institute of Physical Chemistry PAS, Poland
2001 – Professor, College of Science, UKSW, Poland
2003 – Vice-chairmen of Scientific Council, Institute of Physical Chemistry PAS
1991–2001 Short time visits (less than 3 weeks) Harvard, MIT, Brandeis University of Chicago, Ecole Normale Superieure de Paris, Universite Paris Sud, Simon Fraser University, University of Paderborn, Johannes Gutenberg University, Brown University, AMOLF Institute in Amsterdam, Leiden University, Ecole Superieure de Physique et Chimie Industrielles, Universite de Grenoble, Claude Bernard Universite de Lyon, CEA-Saclay, University of Minnesota, Tokyo University, Nagoya University, University of Reading , Universite Libre de Bruxelles, Technical University of Berlin, Samsung Advanced Institute of Technology.

Research areas:

- Soft and living matter: liquid crystals, polymers, microemulsions, Brownian motion, topology and geometry, phase transitions, structure, biochemical networks.

Selected papers

1. Hołyst R., "Landau-Peierls instability, x-ray diffraction patterns and surface freezing in thin smectic films", *Phys. Rev. A*, **44**, 3692 (1991).
2. Góźdź W. and Hołyst R., "Triply periodic surfaces and multiply continuous structures in the Landau model of microemulsions", *Phys. Rev. E*, **54**, 5012 (1996).
3. Hołyst R. and Oswald P., "Confinement induced topological fluctuations in system with internal surfaces", *Phys. Rev. Lett.*, **79**, 1499 (1997).
4. Hołyst R., Poniewierski A., Fortmeier P. and Stegemeyer H., "Coupling of polarization and dislocation in ferroelectric smectic liquid crystal films", *Phys. Rev. Lett.*, **81**, 5848–5851 (1998).
5. Hołyst R. and Przybylski B., "Topological Lifshitz line, off-specular scattering and mesoporous materials", *Phys. Rev. Lett.*, **85**, 130–133 (2000).
6. Fiałkowski M., Aksimentiev A. and Holyst R., "Scaling of the Euler characteristic, surface area and curvatures in the phase ordering/separating systems", *Phys. Rev.Lett.*, **86**, 240 (2001).
7. Graca M., Wieczorek S.A. and Hołyst R., "Polymer domain grown in ordered LC Matrices", *Phys.Rev. Lett.*, **90**, 115504 (2003).
8. Burdy K. and Hołyst R., "Mechanisms of facilitated forget location and the optimal number of molecules in the diffusion search proces", *Phys. Rev. E*, **64**, 011914-1 (2001).

Total number of publications: 120

Alina Ciach, Professor

M.Sc., 1979 – Department of Physics, University of Warsaw
Ph.D., 1986 – Institute of Physical Chemistry, Warsaw
D.Sc., 1994 – Institute of Physical Chemistry, Warsaw
Professor – 2002

Education and training:

1997 – Institute of Theoretical Physics, Trondheim University, Norway (Postdoctoral Research Fellow, Royal Norwegian Council for Scientific and Industrial Research)
1998 – Department of Physics, University of Essen, Germany (Alexander von Humboldt Research Fellow)

Research areas:

- Statistical mechanics of complex systems
- Special fields: self-assembling systems, ionic fluids, effects of boundaries and confinement on structure and thermodynamical properties of simple and complex fluids

Selected papers

1. Stecki J., Ciach A. and Dudowicz J., "Intrinsic properties of the two-point functions of the solid-on-solid interface", *Phys. Rev. Lett.*, **56**, 1482–1484 (1986).
2. Ciach A., Hoye J. and Stell G., "Microscopic model for microemulsion", *J. Phys. A*, **21**, L777–L782 (1988).
3. Diehl H.W. and Ciach A., "Surface critical behavior in the presence of linear or cubic weak surface fields", *Phys. Rev. B*, **44**, 6642–6662 (1991).
4. Ciach A. and Poniewierski A., "Description of the geometrical and topological structure in amphiphilic systems", *Phys. Rev E*, **52**, 596–601 (1995).
5. Ciach A., Maciołek A. and Stecki J., "Critical Adsorption in the Undersaturated Regime. Scaling and Exact Results in the Ising Strip", *J. Chem. Phys.*, **108**, 5913 (1998).
6. Ciach A., Tasinkevych M. and Maciołek A., "Surface phenomena for lamellar phases of microemulsionsEurophys", *Lett.*, **45**, 495–500 (1999).
7. Ciach A. and Stell G., "Effect of competition between Coulomb and dispersion forces on phase transitions in ionic systems", *J. Chem. Phys.*, **114**, 3617 (2001).
8. Babin V., Ciach A. and Tasinkevych M., "Capillary condensation of periodic phases in self-assembling systems", *J. Chem. Phys.*, **114**, 9585 (2001).
9. Ciach A. and Stell G., "Effect of space discretization on phase diagrams in ionic systems; field theoretic approach", *Phys. Rev. Lett.*, **91**, 60601 (2003).

Total number of publications: 57

Jan Stecki, Professor Emeritus

M.Sc., 1952 – Department of Chemistry, University of Warsaw
Ph.D., 1959 – Department of Chemistry, University of Warsaw
D.Sc., 1962 – Institute of Physical Chemistry, Warsaw
Professor, 1972 – Institute of Physical Chemistry, Warsaw

Education and training:

1959–60 – Postdoctoral Research Fellow, Free University of Brussels, Belgium
1962–64 – Senior Research Fellow, University of Southern California, USA
1964 – Research Associate, Rice University, Houston, USA
1969 – Visiting Lecturer, University of Copenhagen, Denmark
1973 – Visiting Professor, University of Trondheim, Norway
1982 – Visiting Research Fellow, P.C.L., Oxford University, UK
1987 – Visiting Fellow, St. Catherine,s College, Oxford University, UK
1992 – Benjamin Meakin Professor, Bristol University, UK
1994 – Visiting Professor, University of Copenhagen, Denmark
1997 – Visiting Professor, University of Cornell, USA

Professional affiliations:

- Polish Chemical Society
- Society for Advancement of Science and Arts (TPKN)

Research areas:

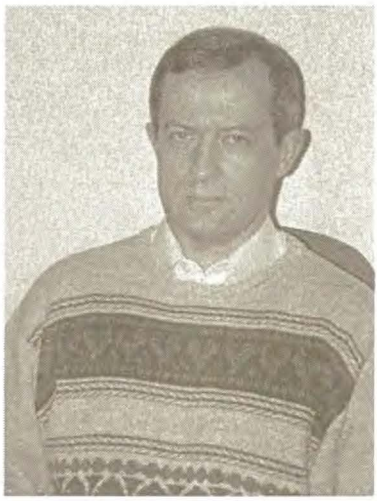
- Statistical mechanics
- Liquids and liquid solutions
- Phase transitions, ordered phases, interfaces

Selected papers

1. Stecki J., "Ionic solvation", *Adv. Chem., Phys.*, **36**, 413–450 (1964).
2. Stecki J. and Taylor H.S., "The areas of equivalence of Bogolyubov and Prigogine's theory of irreversible processes in classical gases", *Rev. Modern Phys.*, **37**, 762 (1965).
3. Poniewierski A. and Stecki J., "Statistical theory of the elastic constants of nematic liquid crystals", *Mol. Phys.*, **38**, 1931–1940 (1979).
4. Maciołek A. and Stecki J., "d = 2 Ising strip with two surface fields solved using the transfer-matrix method", *Phys. Rev. B*, **54**, 1128–1144 (1996).
5. Stecki J., "Variation of the free energy with the interface area: The second derivative". Molecular physics (K.E. Gubbins'issue, 2002); See also *J. Chem. Phys.*, **114**, No.18 (2001).

Total number of publications: 140

Andrzej Poniewierski, Research Associate



M.Sc., 1977 – Department of Physics, University of Warsaw
Ph.D., 1983 – Institute of Physical Chemistry, Warsaw
D.Sc., 1994 – Institute of Physical Chemistry, Warsaw

Education and training:

1983–85 – S.E.R.C., University of Southampton, Great Britain

Research areas:

- Statistical physics of liquid crystals
- Applications of density-functional methods
- Phase transitions and local structure
- Non-uniform systems and interfacial phenomena
- Finite size effects
- Dynamics of liquid crystal films
- Anchoring phenomena
- Structured surfaces

Selected papers

1. Sluckin T.J. and Poniewierski A., "Novel surface phase transition in nematic liquid crystals: wetting and the Kosterlitz-Thouless transition", *Phys. Rev. Lett.*, **55**, 2907–2910 (1985).
2. Poniewierski A. and Sluckin T.J., "The nematic-isotropic transition in a restricted geometry", *Liquid Crystals*, **2**, 281–311 (1987).
3. Poniewierski A. and Hołyst R., "Density-functional theory for nematic and smectic-A ordering of hard spherocylinders", *Phys. Rev. Lett.*, **61**, 2461–2464 (1988).
4. Poniewierski A., "Nematic to smectic-A transition in the asymptotic limit of very long hard spherocylinders", *Phys. Rev. A*, **45**, 5605–5613 (1992).
5. Poniewierski A. and Hołyst R., "Continuous-model description of layer fluctuations in finite smectic systems", *Phys. Rev. B*, **47**, 9840–9843 (1993).
6. Poniewierski A., "Ordering of hard needles at a hard wall", *Phys. Rev. E*, **47**, 3396–3403 (1993).
7. Poniewierski A. and Samborski A., "Smectic-A surface order in a nematic-substrate system", *Phys. Rev. E*, **51**, 4574–4579 (1995).
8. Poniewierski A., Hołyst R., Price A.C. and Sorensen L.B., "Dynamic critical behavior of the Landau-Peierls fluctuations: Scaling form of the dynamic density autocorrelation function for smectic-A films", *Phys. Rev. E*, **59**, 3048–3058 (1999).
9. Poniewierski A., "Shape of the nematic-isotropic interface in conditions of partial wetting", *Liquid Crystals*, **27**, 1369–1380 (2000).
10. Kondrat S. and Poniewierski A., "Uniform and nonuniform textures of a nematic liquid crystal in contact with an inhomogeneous substrate", *Phys. Rev. E*, **64**, 031709-1–031709-9 (2001).

Total number of publications: 50

IV. Department of Chemical Dynamics

Head: Professor Ryszard Duś

The Department was established in 1994 as a result of the reorganization of the Laboratory for Theory of Chemical Kinetics. The research groups in the Department include those which are mainly engaged in theoretical studies and others which are predominantly working experimentally.

1) Investigations of far from equilibrium non-linear chemical systems exhibiting simple and complex periodic oscillations and chaotic behaviors.
2) Modelling of spatio-temporal structures in non-linear: reaction-diffusion and reaction-diffusion-convection systems.
3) Analysis of nonequilibrium effects connected with thermally activated chemical reactions.

The group's scientific output includes over 140 works published in recognised journals *e.g. Phys. Rev., J. Phys. Chem., J. Chem. Phys.*

Experimental research topics include:

1) Application of a set of experimental systems constructed at the Institute and several methods of measurements elaborated here for investigation of surface phenomena occurring in the process of interaction of gases with metals. A significant number of works is connected with the investigation of surface phenomena arising in the process of transition metal hydrides and rare earths metal hydrides formation.
2) Application of Atomic Force Microscopy (AFM) and Tunneling Microscopy (STM) for investigation of surface phenomena "*in situ*" in the course of chosen chemical reactions occurring during interaction of gases with solids.
3) Application of high-pressure mass spectrometer with impulsive ionisation for investigation of energetics, dynamics and reaction of ion clusters in gaseous systems. Investigation by means of this apparatus interactions of ions with molecules occurring in the Earth atmosphere.
4) Use of described phenomenological models for anticipation and description of complex oscillations observed experimentally in non-linear chemical and electrochemical systems.

The scientific output of the experimental group includes over 110 works published in recognised journals *e.g. Langmuir, Surface Sci., Apel. Surface Sci., J. Phys. Chem., Int. J. Mass Spectr.*

At present new topics are approached including, among others:

1. Investigation of the stability of symmetrical solutions in 2 dimensional models of non-linear reaction-diffusion systems.
2. Investigation of influence of fluctuation on the dynamics of model thermochemical system by the master equation method.
3. Attempts at the generalisation of van't Hoff's isobar.
4. Investigation of surface phenomena in the process of transition of thin metal film into a semiconductor in the reaction of creation of terbium and gadolinium trihydrates (problem of the reversible metallic mirrors transmitting light in the visible range).
5. Theoretical and numerical modelling of processes of SHS synthesis for the creation of ceramic materials stable at high temperatures (*e.g.* SiC). Investigation of SHS process parameters determining nanostructural properties of the ceramic materials.
6. Investigation of surface structure and chosen physical properties of thin layers of conducting polymers depending on the manner of their preparation and type of foundation (cooperation with Warsaw University of Technology).
7. Application of AFM and STM microscopy for investigation of adsorption of organic compounds on solids.
8. Application of the high-pressure mass spectrometry for the investigation of ion reactions of biological significance (and in particular energetics and dynamics of their solvation).
9. Application of nonlinear chemical systems for information processing.

Ryszard Duś, Professor

M.Sc., 1959 – Department of Chemistry, Technical University of Warsaw
Ph.D., 1968 – Institute of Physical Chemistry, Warsaw
D.Sc., 1977 – Institute of Physical Chemistry, Warsaw
Professor, 1992 – Institute of Physical Chemistry, Warsaw

Education and training:

1969 – Imperial College of London University, Great Britain
1978 – Wisconsin University, Milwaukee, USA
1996 – University of Liverpool, Great Britain

Research areas:

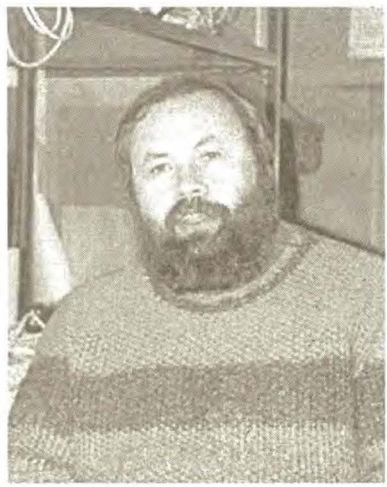
- Surface science: adsorption and reaction of gases on solids. Surface phenomena in the process of hydries and oxides formation. Surface reactions on hydrides (*e.g.* hydrogenation of hydrocarbons, reaction with oxygen

Selected papers

1. Nowicka E. and Duś R., "Hydrogen and Deuterium Adsorption on the Surfaces of Titanium Hydrides and Deuterides", *Langmuir*, **12**, 1520 (1996).
2. Nowakowski R., Kobiela T., Wolfram Z. and Duś R., "Atomic Force Microscopy of Au-Hg alloy formation on thin Au films", *Appl.Surf. Sci.*, **115**, 217 (1997).
3. Duś R., Nowicka E. and Wolfram., "Influence of Oxygen or Methane Preadsorption on Thin Pd Films on Atomic Deuterium Emission from Palladium Deuteride at Low Temperature", *Langmuir*, **14**, 4545 (1998).
4. Duś R. and Nowicka E., "Surface Mediated Formation of Vanadium Hydride", *Langmuir*, **14**, 5487 (1998).
5. Duś R. and Nowicka E., "Deuterium (Hydrogen) Segregation on Palladium Deuteride (Hydride) Surfaces", *Langmuir*, **16**, 789 (2000).
6. Duś R. and Nowicka E., "Surface Phenomena in the Process of Thin Yttrium Hydride Film Formation", *Langmuir*, **16**, 10258 (2000).
7. Duś R. and Nowicka E., "Bivalent Ability for Charge Transfer in Process of Hydrogen Interaction with Surfaces of Transition Metals", *Progress in Surface Sci.*, **67**, 139 (2001).
8. Nowakowski R. and Duś R., "Atomic Force Microscopy Studies of Thin Pd Film Response to Palladium Hydride Formation and Its Reaction with Oxygen", *Langmuir*, **19**, 6750 (2003).
9. Duś R. and Nowicka E., "Atomic Deuterium (Hydrogen) Adsorption on Thin Silver Films", *Progres in Surface Sci.*, **74**, 39 (2003).
10. Duś R., Nowicka E. and Nowakowski R., "Electron Scattering Cross Section on the Surface of Thin Ag and Au Films Induced by Atomic Deuterium Adsorption", *Langmuir*, **20**, 9138 (2004).

Total number of publications: 91

Jerzy Górecki, Professor



M.Sc., 1978 – Department of Physics, Warsaw University

Ph.D., 1984 – Institute of Physical Chemistry, Warsaw

D.Sc., 1994 – Department of Mathematics and Physics, Jagiellonian University, Cracov

since 2003 – teaching professor at the Department of Mathematics and Computer Science, Cardinal Stefan Wyszynski University, Warsaw

Professor, 2004 – Institute of Physical Chemistry, Warsaw

Education and training:

1982–1985 (4 months total) – International Centre for Theoretical Physics, Trieste, Italy

1986–1988 – Department of Chemistry, University of Manchester, UK

1991 – Department of Chemistry, McGill University, Montreal, Canada

1991–1992 – Institute for Molecular Science, Okazaki, Japan

from 1994 – short research visits to Japan (Tokyo Institute of Technology, International Christian University in Mitaka and Kyoto University) and to Italy (La Sapienza, Roma)

Research areas:

- Nonlinear chemical systems and their application in information processing
- Computational chemical kinetics; large scale computer simulations of nonequilibrium chemical systems
- Stochastic effects in chemical systems and their simulations

Selected papers

1. Górecki J. and Pusz W., "Passive states for finite classical systems", *Letters in Mathematical Physics*, **4**, 433 (1980).
2. Górecki J. and Popielawski J., "On the application of the long mean free path approximation to the theory of electron transport properties in liquid noble metals", *J. Phys.*, **F13**, 1197 (1983).
3. Górecki J. and Byers Brown W., "Variational Boundary Perturbation Theory for Enclosed Quantum Systems", *J. Phys.*, **B22**, 2659 (1989).
4. Górecki J. and Eu B.C., "Direct observation of a nonequilibrum velocity distribution in a system with a thermally activated reaction", *J. Chem. Phys.*, **97**, 6695 (1992).
5. Górecki J. and Kitahara K., "Does the structure of an oscillating chemical system oscillate?", *Physica A*, **245**, 64 (1997).
6. Górecki J. and Górecka J.N., "Molecular dynamics simulations of nonequilibrium rate constant in a model exothermic reaction", *Chemical Physics Letters*, **319**, 173 (2000).
7. Sielewiesiuk J. and Górecki J., "Logical Functions of a Cross Junction of Excitable Chemical Media", *J. Phys. Chem.*, **A105**, 8189 (2001).
8. Sielewiesiuk J. and Górecki J., "On complex transformations of chemical signals passing through a passive barrier", *Phys. Rev.*, **E66**, 016212-(1–9) (2002).
9. de Pasquale F., Mecozzi A., Górecki J. and Spagnolo B., "A new stochastic representation for the decay from a metastable state", *Physica*, A **315**, 290–298 (2002).
10. Wakou J., Kitahara K., Litniewski M. and Górecki J., "On Nonequilibrium Spatial Correlations in a Model Chemical Reaction", *Physica*, A **328**, 23–43 (2003).
11. Górecki J., Yoshikawa K. and Igarashi Y., "On chemical reactors that can count", *J. Phys.Chem.*, A **107**, 1664–1669 (2003).
12. Litniewski M. and Górecki J., "On the applicability of the step function nonradiative lifetime model for diffusion controlled reactions", *J. Chem. Phys.*, **119**, 8464–8472 (2003).

Total number of publications: 88

Henryk Wincel, Professor Emeritus

M.Sc., 1958 – Department of Chemistry, Warsaw University
Ph.D., 1965 – Institute of Nuclear Research, Warsaw
D.Sc., 1974 – Institute of Nuclear Research, Warsaw
Professor, 1992 – Institute of Physical Chemistry, Warsaw

Professional experience:

1971/72 – Center of Research of Atoms and Molecules, Laval University, Quebec, Canada
1987; 1998 – Institute of Mass Spectrometry, University of Amsterdam, The Netherlands
1988; 1992 – Dept. of Chemistry and Center for Research in Earth and Space Science, York University, Canada
1993; 1995 – Dept. of Chemistry, The Pennsylvania State University, University Park, USA

Professional affiliations:

- Polish Radiation Association
- Polish Mass Spectrometry Society
- European Society for Mass Spectrometry

Research areas:

- ion/molecule reactions, kinetics and mechanisms
- cluster ions
- ionic processes in the atmosphere
- fullerenes
- ion chemistry of biomolecules

Selected papers

1. Włodek S., Łuczyński Z. and Wincel H., "Gas-phase complexes of NO_2 and NO_3 with SO_2" *Int. J. Mass Spectrom. Ion Phys.*, **49**, 301–309 (1983).
2. Wincel H., Fokkens R.H. and Nibbering N.M.M., "Site of protonation of benzonitrile: hydrogen interchange in the protonated species", *J Am. Soc. Mass Spectrom.*, **1**, 225–232 (1990).
3. Javahery G., Petrie S., Wincel H., Wang J. and Bohme D.K., "Experimental Study of Reactions of the Buckminsterfullerene Cations C_{60}^+, C_{60}^{2+}, and C_{60}^{3+}, with Ammonia and Amines in the Gas Phase", *J. Am. Chem. Soc.*, **115**, 5716–5722 (1993).
4. Wincel H., Mereand E. and Castleman A.W., Jr. "Reactions of N_2O_5 with Protonated Watwer Clusters $H^+(H_2O)_n$, n = 3–30", *J. Phys. Chem.*, **98**, 8606–8610 (1994).
5. Wincel H., " Cluster ions:Gas-phase stabilities of $NO^+(CH_3CN)_n$ and $NO_2^+(CH_3CN)_n$ with n = 1–5 " , *Int. J. Mass Spectrom.*, **203**, 93–100 (2000).
6. Wincel H., Fokkens R.H. and Nibbering N.M.M., " Peptide bond formation in gas-phase ion/molecule reactions of amino acids: a novel proposal for the synthesis of prebiotic oligopeptides", *Rapid Commun. Mass Spectrom.*, **14**, 135–140 (2000).
7. Wincel H., Fokkens R.H. and Niberirg N.M.M., "Gas-phase reactions of NO^+ with Glu and γ-Glu-Met.", *Spectroscopy*, **14**, 4 (2000).
8. Wincel H. and Fokkens R.H., "Gas-phase ion chemistry of Glu/Met systems, Rapid Commun". *Mass Spectrom.*, **16**, 15 (2002).
9. Wincel H., "Gas-phase solvation of Cl^-, NO_2^-, $CH_2NO_2^-$, $CH_3NO_2^-$ and $CH_3NO_4^-$, by CH_3NO_2", Int. *Journal of Mass Spectrometry*, **226**, 341 (2003).

Total number of publications: 92

Andrzej L. Kawczyński, Associate Professor

M.Sc., 1967 – Deparment of Chemistryt, University of Warsaw
Ph.D., 1972 – Institute of Physical Chemistry, Warsaw
D.Sc., 1993 – Institute of Physical Chemistry, Warsaw

Education and training:

1973–74 Institute of Biophysics An USSR, Pushchino, USSR
1989 – Intern. Scool for Advanced Studies, Trieste, Italy
1990–91 – University of Montana, Missoula, USA

Research areas:

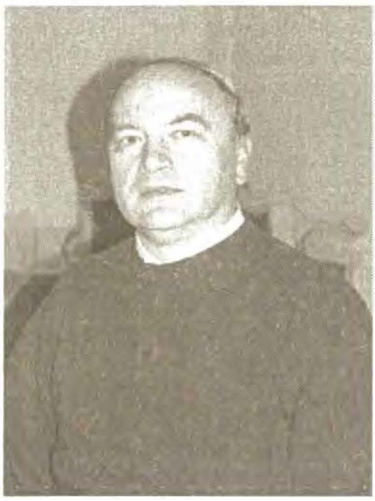
- Nonlinear chemical dynamics
- Theory of dissipative structureas and chaos
- Stochastic approach to dynamics of nonlinear chemical systems
- Microscopic simulations of dissipative structures in chemical sysyems.

Selected papers

1. Zaikin A.N. and Kawczyński A.L., "Spatial effects in a active chemical systems. I. Model of leading center", *J. Non-Equil. Thermodyn.*, **2**, 39 (1977).
2. Kawczyński A.L. and Górski J., "Chemical model of non sustained leading center", *Polish J. Chem.*, **57**, 187 (1983).
3. Kawczyński A.L., "Chemical model of chaos", *Polish J. Chem.*, **58**, 233 (1984).
4. Misiurewicz M. and Kawczyński A.L., "At the other side saddle-node", *Comm. Math. Phys.*, **131**, 605 (1990).
5. Kawczyński A.L. "Chemical reactions – from equilibrium through dissipative stuctures to chaos", WNT, Warsaw 1990, pp. 260 (in Polish).
6. Kawczyński A.L., Comstock W.S. and Field R.J., "The evolution of patterns in a homogeneously oscillating medium", *Physica D*, **54**, 220–234 (1992).
7. Kawczyński A.L., Górecki J. and Nowakowski B., "Microscopic and stochastic simulations of oscillations in a model of chemical system", *J. Phys. Chem.*, **102**, 7113–7122 (1998).
8. Rachwalska M. and Kawczyński A.L., "New types mixed-mode periodic oscillations in the Belousov-Zhabotinsky reaction in a CSTR", *J. Phys. Chem.*, **103**, 3455–3457 (1997).
9. Kawczyński A.L. and Legawiec B., "Coexistence of large amplitude stationary structures in a model of reaction-diffusion system", *Phys. Rev. E*, **63**, 021405(1-12) (2001).
10. Kawczyński A.L. and Legawiec B., "A two-dimensional model of reaction-diffusion system as a typewriter", *Phys. Rev. E*, **64**, 056202(1-4) (2001).

Total number of publications: 97

Bogdan Nowakowski, Associate Professor



M.Sc., 1977 – Department of Physics, University of Warsaw
Ph.D., 1986 – Institute of Physical Chemistry, Warsaw
D.Sc., 2000 – Institute of Physical Chemistry, Warsaw

Education and training:

1989–91 – State University of New York at Buffalo, USA
1992 – State University of New York at Albany, USA
1998 – University P. and M. Curie, Paris, France

Research areas:

- kinetic theory of gases for systems with chemical reactions
- fluctuation effects in nonequilibrium physicochemical systems
- mesoscopic and microscopic Monte Carlo simulations of chemical systems
- dynamics of far-from-equilibrium, nonlinear, dissipative chemical systems

Selected papers

1. Nowakowski B. and Ruckenstein E., "A kinetic approach to the theory of nucleation in gases", *J. Chem. Phys.*, **94**, 1397–1402 (1991).
2. Nowakowski B. and Popielawski J., "The Kinetic Theory of the Effect of Chemical Reaction on Diffusion of a Trace Gas", *J. Chem. Phys.*, **100**, 7602–7609 (1994).
3. Nowakowski B., "Nonequilibrium molecular velocity distribution in binary reactive gaseous mixture", *J. Chem. Phys.*, **109**, 3443–3451 (1998).
4. Lemarchand A. and Nowakowski B., "Perturbation of local equilibrium by a chemical wave front", *J. Chem. Phys.*, **109**, 7028 (1998).
5. Nowakowski B. and Kawczyński A.L., "Master Wquation Approach to Fluctuations in a Model Excitable Spatially Extended Chemical System", *J. Phys. Chem. A*, **102**, 5974 –5979 (1998).
6. Górecki J., Kawczyński A.L. and Nowakowski B., "Master equation and molecular dynamics simulations of spatiotemporal effects in a bistable chemical system", *J. Phys. Chem. A*, **103**, 3200–3209 (1999).
7. Lemarchand A. and Nowakowski B., "Macroscopic effects of the perturbation of the particle velocity distribution in a trigger wave", *Phys. Rev. E*, **62**, 3156–3166 (2000).
8. Nowakowski B. and Lemarchand A., "Stochastic effects in a thermochemical system with Newtonian heat exchange", *Phys. Rev. E*, **64**, 061108 (2001).
9. Nowakowski B. and Lemarchand A., "Sensitivity of explosion to departure from partial equilibrium", *Phys. Rev. E*, **68**, 031105 (2003).
10. Kawczyński A.L. and Nowakowski B., "Master equation simulations of a model of thermochemical system", *Phys. Rev. E*, **68**, 036218 (2003).

Total number of publications: 48

Ewa Nowicka, Associate Professor

M.Sc., 1966 – Faculty of Mathematics and Physics, Warsaw University

Ph.D., 1984 – Institute of Physical Chemistry, Warsaw, Poland

D.Sc., 1999 – Wrocław University, Faculty of Astronomy and Physics, Wrocław, Poland

Education and training:

1982 – CNRS, Saclay, France

1994 – Universite de Marseille, Luminy, France

Research areas:

- Surface science: adsorption and reactions of gases on solids surfaces (metals, hydrides)
- Surface phenomena in the process of hydrides formation
- Surface reactions on metal and metal hydrides surfaces

Selected papers

1. Duś R., Nowicka E. and Wolfram Z., "Surface-mediated formation of vanadium hydrides" *Langmuir*, **14,** 5487–5494 (1998).
2. Duś R. and Nowicka E., "Hydrogen segregation on palladium hydride surface" *Progress in Surface Science*, **59**, 289-300 (1998).
3. Duś R. and Nowicka E., "Surface phenomena in the process of thin yttrium hydride film formation"*Langmuir*, **16**, 10258–10264 (2000).
4. Duś R. and Nowicka E.,"Bivalent ability for charge transfer in process of hydrogen interaction with surfaces of transition metals"*Progress in Surface Science,* **67,** 139–154 (2001).
5. Duś R. and Nowicka E., "Hydrogen distribution between the surface and the bulk of thin nickel film at low temperatures"*Vacuum*, **63**, 249–256 (2001).
6. Duś R. and Nowicka E.,"Surface mediated yttrium deuteride formation", *Surface Science,* **507/510**, 819–824 (2002).
7. Duś R. and Nowicka E.,"Atomic deuterium (hydrogen) adsorption on thin silver films"*Progress in Surface Science,* **74,** 39–56 (2003).
8. Duś R., Nowicka E. and Nowakowski R., "Electron scattering cross-section on the surface of thin Ag and Au films induced by atomic deuterium adsorption" *Langmuir*, **20**, 9138–9143 (2004).

Total number of oublications: 49

Andrzej Cukrowski, Research Associate

M.Sc., 1959 – Department of Chemistry, Technical University of Warsaw
Ph.D., 1967 – Institute of Physical Chemistry, Warsaw
D.Sc., 1994 – Institute of Physical Chemistry, Warsaw

Education and training:

1971 – FOM Institute of Atomic and Molecular Physics, Amsterdam, The Netherlands
1991–92 – Department of Chemistry, Chemical Engineering and Material
Sciences, University of Minnesota, Minneapolis, USA

Professional affilations:

- Polish Chemical Society

Research areas:

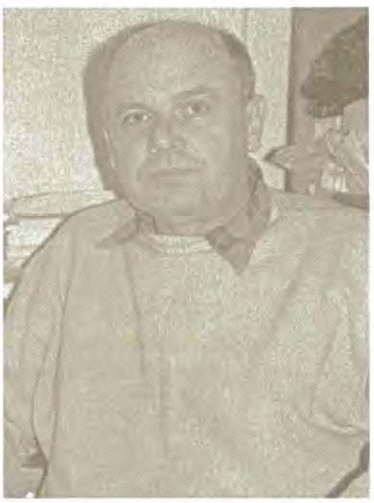
- Description of transport processes in continueous media within the formalism of non-equilibrium thermodynamics with emphasis of the role of reference frames
- Non-equilibrium solvation numbers in liquid electrolyte solutions
- Kinetic theory of non-equilibrium processes in gases (Boltzmann equation) with introduction of simple models of cross sections
- Application of the kinetic theory of gases for description of non-equilibrium effects connected with proceeding of chemical reactions
- Problems of different temperatures of reacting components and of negative Arrhenius activation energy
- Processes of energy relaxation in gases
- Performing of computer simulations giving numerical results for comparisons with analytical results derived within the kinetic theory

Selected papers

1. Baranowski B. and Cukrowski A.S., "Transfer processes in liquid isothermal solutions of binary electrolytes", *Z. phys. Chem.*, **228**, 292–309 (1965).
2. Cukrowski A.S., "On rotational relaxation of spherical gas molecules", *Chem. Phys. Lett.*, **12**, 514–517 (1972).
3. Cukrowski A.S., "Transport coefficients and solvation numbers in liquid electrolyte solutions under isothermal conditions", *J. Non-Equil. Thermodyn.*, **2**, 69–84 (1977).
4. Cukrowski A.S. and Popielawski J., "The dependence of the rate constant of chemical reaction on density derived from the generalized Enskog equation for dense gases", *J. Chem. Phys.*, **78**, 6584–6587 (1983).
5. Cukrowski A.S., Popielawski J., Schmidt R. and Stiller W., "Nonequilibrium contributions to the rate of chemical reaction in the Lorentz gas: A comparison of perturbation and numerical solutions of the Boltzmann equation", *J. Chem. Phys.*, **89**, 197–203 (1988).
6. Cukrowski A.S. and Popielawski J., Lihong Qin, Dahler J.S., "A simplified theoretical analysis of nonequilibrium effects in bimolecular gas phase reactions", *J. Chem. Phys.*, **97**, 9036–9093 (1992).
7. Cukrowski A.S., Fritzsche S. and Stiller W., "Synergistic effects in bimolecular reactions in a dilute gas" *Chem. Phys.*, **181**, 7–14 (1994).
8. Cukrowski A.S., "The role of products and a reverse reaction in analysis of nonequilibrium effects in a bimolecular chemical reaction in a dilute gas" *Physica A*, **275**, 134–151 (2000).
9. Cukrowski A.S., Fritzsche S. and Fort J., "Nonequilibrium effects on the rate of bimolecular chemical in dilute gas", *Chem. Phys. Lett.*, **341**, 585–593 (2001).
10. Cukrowski A.S., Fritzsche S. and Cukrowski M.J. Jr., "A large nonequilibrium effects of decrease of the bimolecular chemical reaction rate in a dilute gas", *Chem. Phys. Lett.*, **379**, 193–201 (2003).

Total number of publications: 70

Wojciech Lisowski, Research Associate



M.Sc., 1972 – University of Warsaw, Warsaw, Poland
Ph.D., 1980 – Institute of Physical Chemistry, Warsaw, Poland
D.Sc., 1996 – Institute of Physical Chemistry, Warsaw, Poland

Education and training:

1978 – J. Heyrovsky Institute of Physical Chemistry, Czechoslovak Academy of Sciences, Prague, Czechoslovakia
1980 – Twente University of Technology, Enschede, The Netherlands
1986 – Twente University of Technology, Enschede, The Netherlands
1989–1991 – University of Twente, Enschede, The Netherlands
1999 – Institut für Physikalische und Theoretische Chemie der Universität Bonn, Bonn, Germany
2001 – University of Twente, Enschede, The Netherlands

Research areas:

- Adsorption and reaction of gases on solids
- Surface and interface studies of solid state materials

Selected papers

1. Lisowski W. and Duś R., "Adsorption of Alkanes and Their Coadsorption with Hydrogen on Evaporated Palladium Thin Films", *Surface Sci.*, **107**, 51 (1981).
2. Lisowski W., Nowicka E., Wolfram Z. and Duś R., "Atomic Hydrogen Desorption from Thin Palladium Hydride Films", *Appl. Surface Sci.*, **31**, 157 (1988).
3. Lisowski W., "Kinetics and Thermodynamics of Hydrogen Interaction with Thin Cobalt Films", *Appl. Surface Sci.*, **33**, 399 (1988/89).
4. Lisowski W., Hemmes H., Jäger D., Stöver D. and van Silfhout A., "Interaction Between Plasma Sprayed YBaCuO and Nimonic Substrates", *Appl. Surface Sci.*, **662**, 13 (1992).
5. Lisowski W., "Low-Temperature Interaction of Hydrogen with Methane Precovered Thin Palladium Films", *Surface Sci.*, **312**, 157 (1994).
6. Duś R., Lisowski W., Nowicka E. and Wolfram Z., "Oxygen interaction with palladium hydride and titanium hydride surfaces", *Surface Sci.*, **322**, 285 (1995).
7. van den Berg A.H.J., Lisowski W. and Smithers M., "SEM and AES depth profile studies of thin titanium and titanium oxide films covered by nanoscale evaporated Au layers", *Fresenius J. Anal. Chem.*, **365**, 231 (1999).
8. Lisowski W., "Flow Technique for Measuring the Sticking Probabilities of Simultaneously Adsorbed Gases on Metal Films: Application to the Simultaneous Adsorption of Deuterium and Nitrogen on Thin Iron Film at 78 K", *Vacuum*, **54**, 13 (1999).
9. Lisowski W., van den Berg A.H.J., Leonard D. and Mathieu H.J., "Characterization of titanium hydride films covered by nanoscale evaporated Au layers: ToF-SIMS, XPS and AES depth profile analysis", *Surf. Interface Anal.*, **29**, 292 (2000).
10. Lisowski W., Keim E.G. and Smithers M.A., "High-temperature interaction of nitrogen with thin iron films: Thermal desorption kinetics studies combined with microstructure analysis of Fe-N films", *J. Vac. Sci. Tech. A*, **21(3)**, 545 (2003).

Total number of publications: 50

V. Department of Catalysis on Metals

Head: Professor Zbigniew Karpiński

Department of Catalysis on Metals was established in 1964 as a result of the transformation of the Laboratory for Surface and Structural Research which was initially a part of the Department of Physical Chemistry of Electrode Processes. The Department has achieved a lot both in fundamental and applicative research (among others, for "Blachownia Śląska" and "Mazowieckie Zakłady Rafineryjne i Petrochemiczne" in Płock).

The Department's research techniques were systematically developed with a number of modern methods of physicochemistry of surfaces including: low energy electron diffraction (LEED), Auger Electron Spectroscopy (AES), measurement of work function from a metal. The development of this methodology, among others, in respect to a quantitative composition of surface, supported by intensified theoretical research resulted in the creation of a new department specialising in electron spectroscopies.

In recent years the Department's activity has been concentrated on the complex research of catalysts of the following types Pd/SiO_2, Pd/C, $Pd-Au/SiO_2$ and Pd-Au/C. A simulation of a cluster structure by the molecular dynamic method enabled the interpretation of x-ray measurements conducted *in situ* in the course of chemical reactions for Pd/SiO_2 and Pd/C systems The influence of the sizes of palladium crystallites on the mechanism and kinetics of the selective hydrogenation of acetylene in a mixture with ethylene on palladium catalysts was investigated and a generalised kinetic model of this reaction was described. Works concerning the reduction of Pd/SiO_2 systems showed that already in a relatively low temperature of reduction the palladium-silica interaction results in the formation of palladium silicides what has a considerable influence on catalytic properties in the reaction of conversion of saturated hydrocarbons.

In the context of environmental protection a great significance should be attached to works conducted on catalytic hydrodechlorination of freon R-12 (CCl_2F_2) on Pd-Au/C catalysts. Method of production of highly selective catalysts was described in order to remove chlorine from the freon molecule and the role of the incorporation of carbon to palladium in the course of the reaction was revealed.

Current topics studied in the Department include:

1. Structure versus reactivity of highly dispersed metals and the development of methods of characterisation of catalysts in highly selective catalysis in heterogeneous systems.
2. Structure of highly dispersed solids (nanocrystallites).
3. Kinetics of autooxidation (chain oxidation reaction) of sulphur dioxide in the aspect of the influence of this reaction on the environment. This topic is a continuation of the research conducted in the framework of the Department of Process Kinetics which was joined together with Department V in 2004.

The following new topics are going to be approached:

1. Investigation of metal-support interactions in catalytic systems with palladium,
2. Expanding investigations with the polycrystalline diffractometry method and X-ray spectrometry to include highly dispersed Pd-Ni and Pd-Ag systems,
3. Interpretation of diffraction phenomena (XRD) and absorption (EXAFS) on nanocrystals on the basis of atomistic simulations,
4. Catalytic hydrodechlorination of organic compounds,
5. Expanding research on interactions of sulphur-oxygen radicals to include biologically active substances like, *e.g.* vitamins and enzymes (SO_2 as a food preservative) and substances of biological origin like, *e.g.* dimethyl sulfide, DMS (as a precursor to SO_2 on sea areas).

Zbigniew Karpiński, Professor

M.Sc., 1966 – Dept. of Chemistry, Warsaw Technical University
Ph.D., 1972 – Institute of Physical Chemistry, Warsaw
D.Sc., 1990 – Institute of Physical Chemistry, Warsaw
Professor, 1997 – Institute Physical Chemistry, Warsaw

Education and training:

1973–74 – Dept. of Chemistry, University College, Dublin, Ireland (Postdoctoral Fellow)

1975, 1976 – Institute of Isotopes of HAS, Budapest, Hungary (exchange)

1981–82 – Dept. of Chemistry, Northwestern University, Evanston, Ilinois (Fulbright Fellow)

1988, 1991 – Dept. of Chemistry, Northwestern University, Evanston, Illinois (Research Fellow)

1995 – Dept. of Chemical Engineering, University of Pittsburgh (Visiting Professor)

Professional affiliations:

- Department of Catalysis on Metals
- Polish Catalysis Club (vice-chairman from 1993)
- Polish Chemical Society
- Professor of chemistry at Cardinal Stefan Wyszyński University in Warsaw, Faculty of Mathematics and Natural Sciences, School of Sciences, from 2001 (chemistry chair, from 2003)
- Member of Editorial Board of Applied Catalysis A: General (1997–2001)
- Member of the Scientific Committee of Chemistry of PAS (from 2003)

Research areas:

- Structure and catalytic reactivity of highly dispersed metals
- Catalysis on supported metal alloys
- Kinetics and mechanism of hydrocarbon reactions
- Environmental catalysis (hydrodechlorination of CFCs and VOCs)

Selected papers

1. Karpiński Z., "Catalysis by Supported, Unsupported and Electron-Deficient Palladium", *Adv. Catal.*, **37**, 45–100 (1990).
2. Karpiński Z., Gandhi S.N. and Sachtler W.M.H., "Neopentane Conversion Catalyzed by Pd in L Zeolite: Effects of Protons, Ions and Zeolite Structure", *J. Catal.*, **141**, 337–346 (1993).
3. Juszczyk W., Karpiński Z., Łomot D., Pielaszek J. and Sobczak J.W., "Pd-Au/SiO_2: Characterization and Catalytic Activity", *J. Catal.*, **151**, 67–76 (1995).
4. Karpiński Z., Early K. and d'Itri J.L., "Catalytic Hydrodechlorination of 1,1-Dichlorotetrafluoroethane by Pd/Al_2O_3", *J. Catal.*, **164**, 378–386 (1996).
5. Malinowski A., Juszczyk W., Bonarowska M., Pielaszek J. and Karpiński Z., "Pd-Re/Al_2O_3: Characterization and Catalytic Activity in Hydrodechlorination of CCl_2F_2", *J. Catal.*, **177**, 153–163 (1998).
6. Malinowski A., Łomot D. and Karpiński Z., "Hydrodechlorination of CH_2Cl_2 over Pd/γ-Al_2O_3. Correlation with Hydrodechlorination of CCl_2F_2 (CFC-12)", *Appl. Catal. B: Environmental*, **19**, L79–L86 (1998).
7. Bonarowska M., Pielaszek J., Juszczyk W. and Karpiński Z., "Characterization of Pd-Au/SiO_2 Catalysts by X-Ray Diffraction, Temperature-Programmed Hydride Decomposition and Catalytic Probes", *J. Catal.*, **195**, 304–314 (2000).
8. Bonarowska M., Malinowski A., Juszczyk W. and Karpiński Z., "Hydrodechlorination of CCl_2F_2 (CFC-12) over Silica-Supported Palladium-Gold Catalysts", *Appl. Catal. B: Environmental*, **30**, 187–193 (2001).

Total number of publications: 104

Jerzy Pielaszek, Professor

M.Sc., 1964 – Faculty of Physics, Warsaw University
Ph.D., 1972 – Institute of Physical Chemistry, Warsaw
D.Sc., 1995 – Institute of Physics, Warsaw University of Technology
Professor 2004 – Institute of Physical Chemistry, Polish Acad. of Sci.

Education and cooperation training:

1972 – Commissariat B L'Enérgie Atomique, Fontenay-aux-Roses, France
1974 – University College of Wales, Aberystwyth, Walia, UK
1981–1983 – Nortwestern University, Evanston, USA
2001, 2002, 2003, 2004, 2005 – Université Henri Poincaré, Nancy, France

Professional affiliations:

- Polish Crystallographic Association
- Polish Chemical Society

Research areas:

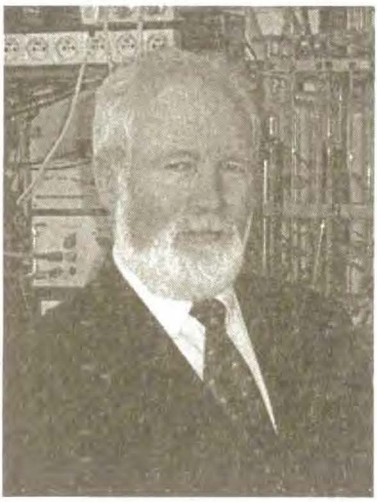
- X-Ray diffraction
- X-ray crystallography in material science
- Structure of nanocrystalline systems (supported catalysts, carbon-metal systems, materials for batteries).

Selected papers

1. Pielaszek J., "X-Ray Powder Diffractometry in Studies of Solid Carbons" – *Fuel*, **73**, 1792–1796 (1994).
2. Mierzwa B. and Pielaszek J., "Smoothing of low intensity, noise data by Fourier filtering: application to supported metal catalyst studies", *J. Aplied Cryst.*, **30**, 544–546 (1997).
3. Laberty Ch., Pielaszek J., Alphonse P. and Rousset A., "Characterization of Nonstoichiometric Nickel Manganite Spinels by Temperature Programmed Reduction", *Solid State Ionics*, **110**, 293–302 (1998).
4. Jak M.J.G., Kelder E.M., Kaszkur Z.A. and Pielaszek J., "Li-Ion Conductivity of BPO_4-Li_2O; The Relation Between Crystal Structure and Ionic Conductivity", *Solid State Ionics*, **119**, 159–164 (1999).
5. Mierzwa B., Kaszkur Z., Moraweck B. and Pielaszek J., "In-situ EXAFS Study of the Alloy Catalyst Pd-Co(50%/50%)/SiO_2", *Journal of Alloys and Compounds*, **286**, 93–97 (1999).
6. Pielaszek J., Kaszkur Z. and Mierzwa B., "X-Ray studies of nanomaterials: theory and experiment", Applied Crystallography, Proceedings of the XVIII Conference (September 2000, Wisła, Poland, Eds. H. Morawiec, D. Stróż), World Scientific pp. 21–27 (2001).
7. Nowakowski R., Pielaszek J. and Duś R., "Surface mediated Ag-Hg alloy formation under ambient and vacuum conditions – AFM and XRD investigations" *Application Surf. Sci.*, **199**, 40–51 (2002)
8. Jedynak A., Szmigiel D., Raróg W., Zieliński W., Pielaszek J., Dłużewski P. and Kowalczyk Z., " Potassium-promoted carbon-based iron catalysts for ammonia synthesis. Effect of Fe dispersion", *Catal. Letters*, **81**, 213–219 (2002).
9. Lisovytskiy D., Kaszur Z., Baumer N.V., Pielaszek J., Molenda M., Dziembaj R., Marzec J., Molenda J., Dygas J. and Krok F., "Phase Transformation of Nanocrystalline Lithium Manganese Spinels Produced by Low and High Temperature Methods", *Molecular Phys. Reports*, **35**, 26–30 (2002).
10. Pielaszek J., "X-Ray Diffraction from Nanostructured Materials" chapter in: Nanocrystalline Metals and Oxides, Selected Properties and Application, Eds. P. Knauth, J. Schoonman, Kluwer Academic Publishers, (2002).
11. Juszczyk W., Karpiński Z., Łomot D. and Pielaszek J., "Transformation of Pd/SiO2 into palladium silicide during reduction at 450 and 500°C". *J. Catal.*, **220**, 299–308 (2003).
12. Lisovytskiy D., Kaszur Z., Baumer N.V., Pielaszek J., Marzec J., Molenda J., Dygas J., Kopeć M. and Krok F., "Phase Transformation in Li-Mn-O spinels synthesized by sol-gel method", *Mater. Sci. Forum*, **443–444**, 311–314 (2004)

Total number of publications: 94

Andrzej G. Borodziński, Research Associate



M.Sc., 1966 – Department of Chemistry, Technical University of Warsaw

Ph.D., 1973 – Institute of Physical Chemistry, Warsaw

D.Sc., 2003 – Technical University of Szczecin, Szczecin

Education and training:

- 1977–1978 Queen's University, Kingston, Ontario, Canada

Professional affiliations:

Polish Catalysis Club

Research areas:

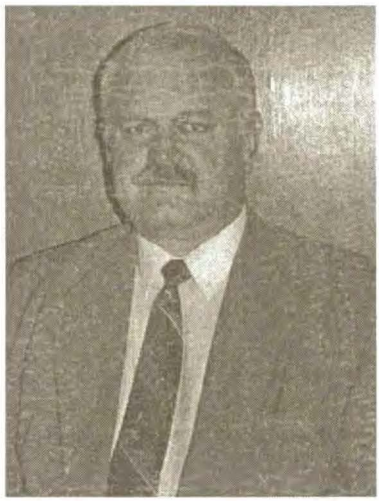
- Complex catalysts for ammonia synthesis
- Solubility of gases in molten salts
- Catalytic cracking on molecular sieves
- Wide experience in selective acetylene – hydrogenation process (involved with the process since 1974: cooperation with industry and fundamental studies, patents and their industrial application in Polish industry)

Selected papers

1. Borodziński A., Duś R., Frąk R., Janko A. and Palczewska W., "A Study of the Role of the Pd-Hydride Phase in the Activity and Selectivity of Pd Catalysts in Acetylene Hydrogenation", *Proc. VI Int. Congress on Catalysis*, London 1976, Paper A7, Eds. G.C. Bond, P.B. Wells and F.C. Tompkins, The Chemical Society, London, p. 150–167 (1977).
2. Zieliński J. and Borodziński A., "A Novel-Design Camera for Simultaneous X-Ray and Kinetic Studies", *Appl. Catalysis*, **13**, 305–310 (1985).
3. Borodziński A., Corma A. and Wojciechowski B.W., "The Nature of the Active Sites in The Catalytic Cracking of Gas-Oil", *Canadian J. Chem. Eng.*, **58**, 219–229 (1980).
4. Borodziński A. and Gołębiowski A., "Surface Heterogeneity of Supported Palladium Catalyst for the Hydrogenation of Acetylene-Ethylene Mixtures", *Langmuir*, **13**, 883–887 (1997).
5. Borodziński A. and Bonarowska M., "The relation between crystallite size and dispersion on supported metal catalysts", *Langmuir*, **13**, 5613–5620 (1997).
6. Borodziński A., "Hydrogenation of acetylene-ethylene mixtures on commercial palladium catalyst", *Catal. Lett.*, **63**, 35–42 (1999).
7. Borodziński A. and Cybulski A., "The kinetic model of hydrogenation of acetylene-ethylene mixtures over palladium surface covered by carbonaceous deposits", *Appl. Catal. A*, **198**, 51–66 (2000).
8. Borodziński A. and Gołębiowski A., "Surface Heterogeneity of Supported Palladium Catalyst for the Hydrogenation of Acetylene-Ethylene Mixtures", *Langmuir*, **13**, 883–887 (1997).
9. Borodziński A. and Bonarowska M., "The relation between crystallite size and dispersion on supported metal catalysts", *Langmuir*, **13**, 5613–5620 (1997).

Total number of publications and patents: 29

Lech Gmachowski, Research Associate



M.Sc., 1971 – Department of Chemistry, Technical University of Warsaw, Poland

Ph.D., 1980 – Institute of Physical Chemistry, Warsaw

D.Sc., 1994 – Faculty of Chemical and Process Engineering, Technical University of Warsaw, Poland

Education and training:

1987–88 – Department of Chemical Engineering, Nagoya University, Japan

Research areas:

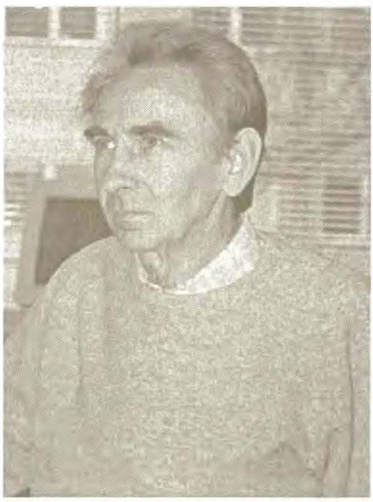
- Aggregation kinetics
- Aggregate structure
- Aggregation of metal particles on catalyst support
- Solution properties of macromolecules and bioparticles
- Hydrodynamics of aggregated systems

Selected papers

1. Gmachowski L., "A new method of polymer molecular weight determination based on the permeable sphere model", *Polymer J.*, **18**, 783–789 (1986).
2. Gmachowski L., "A new relative method of polymer molecular weight determination", *Polymer J.*, **18**, 791–794 (1986).
3. Gmachowski L., "A universal curve representing the concentration and molecular weight dependences of sedimentation coefficient", *Polymer J.*, **22**, 771–775 (1990).
4. Gmachowski L., "Mechanism of shear aggregation", *Water Research*, **29**, 1815–1820 (1995).
5. Gmachowski L., "Hydrodynamics of aggregated media", *J. Colloid Interface Sci.*, **178**, 80–86 (1996).
6. Gmachowski L., "Estimation of the dynamic size of fractal aggregates", *Colloids Surfaces A: Physicochem. Eng. Aspects*, **170**, 209–216 (2000).
7. Gmachowski L., "A method of maximum entropy modeling the aggregation kinetics", *Colloids Surfaces A: Physicochem. Eng. Aspects*, 176, 151–159 (2001).
8. Gmachowski L., "Intrinsic viscosity of bead models for macromolecules and bioparticles", *European Biophysics J.*, **30**, 453–456 (2001).
9. Gmachowski L., "Binary collision growth of supported metal catalyst particles", *Colloids Surfaces A: Physicochem. Eng. Aspects*, **197**, 183–191 (2002).

Total number of publications: 38

Jerzy P. Zieliński, Research Associate



M.Sc., 1964 – Department of Chemistry, Technical University of Warsaw
Ph.D., 1969 – Institute of Physical Chemistry, Warsaw
D.Sc., 1998 – Institute of Physical Chemistry, Warsaw

Education and training:

1971 – Institute of Chemical Process Fundamentals, Prague (three month), Czech Republic
1973 – Institute of Catalysis, Novosibirsk, Russia
1974–1975 McMaster University, Hamilton, Ontario, Canada

Professional affiliation:

- Polish Catalysis Club

Research area:

- Characterization of supported metal catalysts by chemical methods
- Effect of support and promoters on activity and selectivity of metal catalysts
- Hydrogenation of carbon oxides and steam reforming of methane
- Hydrogenation of nitrogen

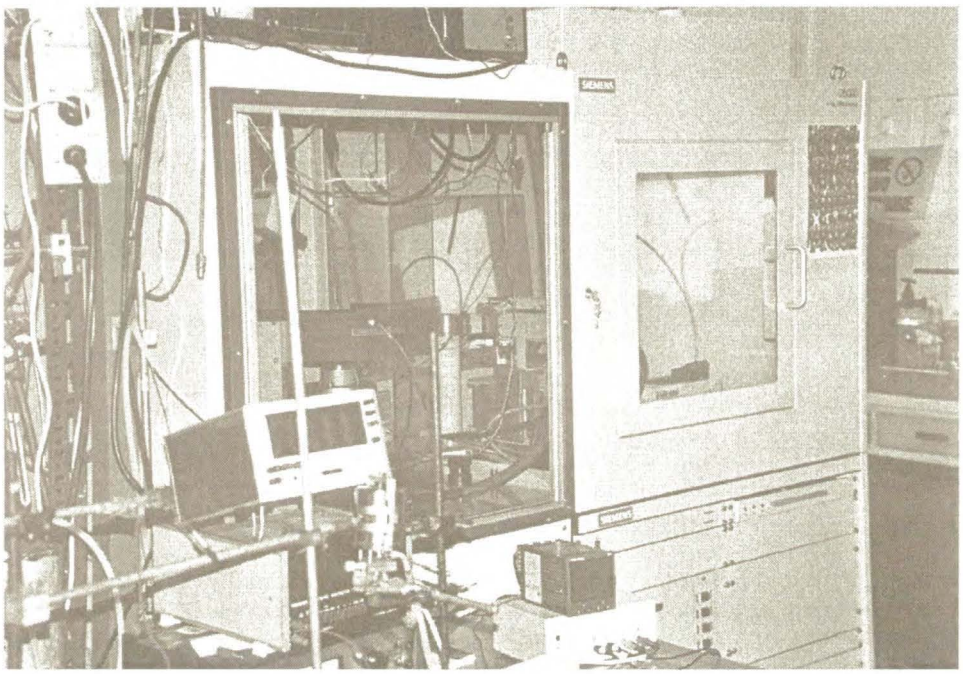
Selected papers

1. Zieliński J., "Morphology of nickel/alumina catalysts", *J. Catal.*, **76**, 157 (1982).
2. Zieliński J., "Morphology of coprecipitated Ni/Al_2O_3 catalysts with low alumina content", *Appl. Catal.*, **94**, 107 (1993).
3. Zieliński J., "Effect of water on the reduction of nickel/alumina catalysts. Catalyst characterization by temperature-programmed reduction", *J. Chem. Soc., Faraday Trans.*, **93(19)**, 3577–3580 (1997).
4. Kowalczyk Z., Jodzis S., Raróg W., Zieliński J. and Pielaszek J., "Effect of potassium and barium on the stability of a carbon-supported ruthenium catalyst for the synthesis of ammonia", *Appl. Catal. A: General*, **173**, 153 (1998).
5. Szmigiel D., Bielawa H., Kurtz M., Hinrichsen O., Muhler M., Raróg W., Jodzis S., Kowalczyk Z., Znak L. and Zieliński J., "The Kinetics of Ammonia Synthesis over Ruthenium-Based Catalysts: The Role of Barium and Cesium", J. *Catal..*, **205**, 205 (2002).
6. Zieliński J., Znak L. and Kowalczyk Z., "Adsorption of dinitrogen and its hydrogenation on a fused iron catalyst for ammonia synthesis", *Langmuir.*, **18(26)**, 10191 (2002).

Total number of publications: 53

Laboratory of X-ray Powder Diffractometry and Spectrometry

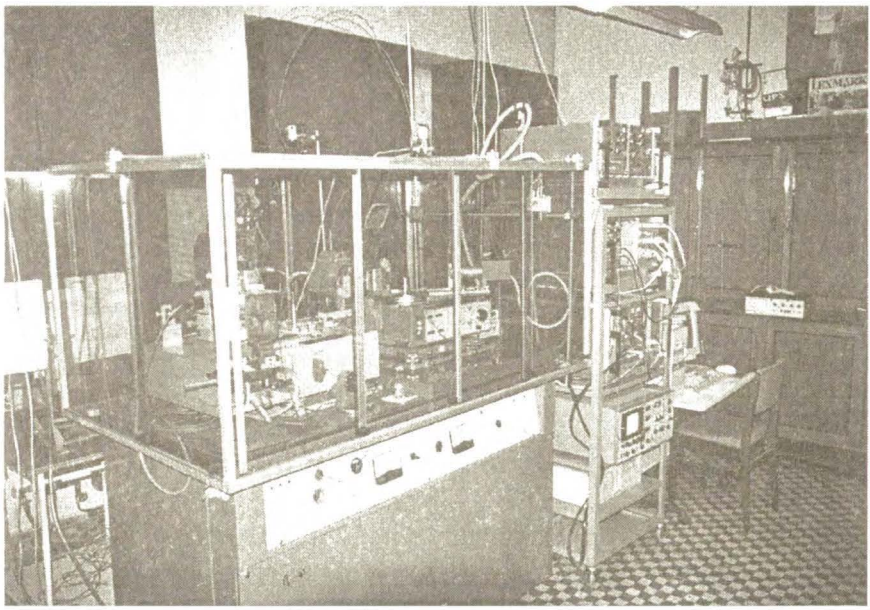
Head: Dr. Zbigniew Kaszkur



Laboratory of X-Ray Powder Diffraction and Spectrometry has been created in 1994 in the Institute of Physical Chemistry (Warsaw, Poland) within the Department of Catalysis on Metals. The laboratory engages itself in a range of projects involving widely understood phase analysis and Rietveld refinement of structural data based on high resolution powder diffraction patterns as well as dynamical and kinetic studies *in-situ* in variable, controlled atmosphere and programmed temperature (from R.T. upto ~600°C).

The laboratory specialises also in the analysis of the state of organization of quasi-amorphous materials. Our long time experience and expertise was focused on the studies of such materials using wide angle X-Ray Powder Diffraction as well as Radial Distribution Function method (RDF). We have also developed many numerical techniques to study highly dispersed solids (transition metals) deposited on supports (SiO_2, Al_2O_3). These techniques include reliable background estimation in the XRD pattern, data smoothing procedures and quantitative analysis oriented towards *in-situ* studies. Recently we have developed a series of analytic tools allowing insight into the structure and dynamics of nanocrystalline metallic particles in a chemical reaction environment. These techniques are developed and verified on the basis of molecular simulations.

Besides the above , the laboratory offers also orientation and cutting of metal single crystals along desired crystallographic plane.



The laboratory has the following equipment:

- X-Ray Diffractometer D5000 (Siemens) equipped with Goebel optics (Cu Kα),
- X-Ray Diffractometer Geigerflex (Rigaku-Denki)
- Position Sensitive Detector CPS 120 (Inel), covering 120° arc, with channel separation ~0.03°
- Position Sensitive Detector type Brown 50 M, with position resolution < 80 μm, set up also in scanning mode
- range of our own design chemical reactors- X-ray cameras developed for *in-situ* X-ray diffraction studies in a controlled atmosphere in flow of selected gases, mixtures of vapors of particular partial pressures at selected, programmed (fully computer controlled) temperatures

The laboratory is cooperating with and offering services and expertise to different scientific and industrial partners, among them:

- Laboratories of the Institute of Physical Chemistry, Polish Academy of Sciences
- Institute of Organic Chemistry, Polish Academy of Sciences
- Warsaw University of Technology
- Jagiellonian University
- POLFA farmaceutical company

Contact persons:

Dr. Zbigniew Kaszkur; zbig@ichf.edu.pl

Laboratory web page:

(http://ichf.edu.pl/res/res_en/lab_xrd/LabXRD.html)

VI. Department of Electrochemistry, Corrosion and Applied Surface Science

Head: Professor Tadeusz Zakroczymski

The Department was established in 2003 as a result of a unification of the Department of Electrochemistry and Corrosion, which had been a part of the structure of the Institute since 1962, and the Department of Applied Surface Science. The Department conducts research of surface processes on metals and alloys that result from the influence of liquid (electrochemical processes) and gaseous environments, conducts theoretical research in the scope of electron spectroscopy, collects and describes phase equilibria data.

The most important achievements of the research teams in recent years are as follows:

- Wide research has been done on kinetics and mechanism of corrosion and passivation of many metal/environment systems. Phenomena of pitting, stress corrosion cracking and hydrogen embrittlement have been investigated in detail.
- A collective work on various aspects of corrosion and hydrogen in metals was published: "Corrosion of Metals and Hydrogen-Related Phenomena", (Ed.: J. Flis), PWN-Elsevier, Warszawa-Amsterdam, 1991.
- Effective methods of protection against corrosion in many technical equipments and industrial installations have been developed. Corrosion inhibitor "SKOLPAN" (awarded the title of Vice-Master of Technology NOT (*Polish Federation of Engineering Associations*)) was worked out and it was applied in Mazowieckie Zakłady Rafineryjne i Petrochemiczne in Płock, Rafineria Trzebinia and Zakłady Koksochemiczne "Hajduki".
- Description and experimental verification of formalism of electron transport in solids was carried on the basis of the approximate solution of the Boltzmann kinetic equation and the extensive Monte Carlo simulations.
- It was shown that the assumption of the uniform distribution of ionisation in surface area, generally made in Auger electron spectroscopy, may be untrue in some analytical situations. The ways of determination of this distribution were suggested.
- A new parameter, the so-called Depth Distribution Function, was introduced for the description of photoelectrons and Auger electrons. This function is now in a general use. ISO and ASTM suggested standard definitions of this quantity. The application of this function to determine concentration profile in the surface area was proposed (A. Jabłoński).
- Determination of a parameter called the electron attenuation length was described. Definitions and expressions of this parameter for various uses of XPS spectroscopy were given (A. Jabłoński, C.J. Powell, "The Electron Attenuation Length Revisited", Surface Science Reports, 47,33 (2002).
- New methods were proposed for critical evaluation and prediction of vapour-liquid and liquid-liquid equlibria used in technological processes and environmental protection. The data calculated with the use of these methods equal the best experimental data and are treated by the IUPAC as the reference data.

Current research topics include the following issues:

- Modification of iron surface layers, unalloyed and alloyed steels through plasma nitriding and/or chemical processing (oxidation and phosphatizing) in order to increase the corrosion resistance of these materials. Investigation of anode behaviour of modified layers and their interaction with hydrogen. Investigation of the synergism of an interaction of nitrogen and molybdenum in austenitic steels in order to increase their pitting resistance.
- Determination of the permeation and desorption rate of hydrogen by the electrochemical technique and description of a procedure enabling qualitative and quantitative characteristics of the entry, transport (diffusion), absorption and trapping of hydrogen in metals. Research on the effect of a long-term cathodic polarisation of iron and its alloys to explain the discovered phenomenon of the surface activation for hydrogen entry, as a result of this polarisation. Changes in the structure of steels during a long-term exploitation and their influence on hydrogen embrittlement. Transport and hydrogen behaviour in aluminium and its alloys and intermetallic compounds with titanium, nickel and iron.

- Theoretical works aiming at possibly exact description of the transport of photoelectrons and Auger electrons in solids, and experimental verification of reliability of the worked out theoretical models.
- Theoretical and experimental works connected with determination of parameters necessary to describe the transport of electrons (a mean free path of electrons, a mean transport path, elastic collision cross-sections).
- Determination of algorithms for analytical applications of electron spectroscopies.
- Distribution and control of effectiveness of the developed electron spectroscopy software in other laboratories.
- Determination of vapour-liquid and liquid-liquid equilibria on the basis of the thermodynamic data bank.

New research topics currently approached:

1. Preparation and electrochemical properties of nanolayers of alkoxysilanes and conductive polymers designated for the corrosion protection.
2. Explanation which of the factors (stress or dynamic strain) is responsible for the initiation and process of corrosion cracking (hydrogen embrittlement) of iron and its alloys stretched in the presence of hydrogen.
3. Influence of multiplex layers of intermetallic compounds on the basis of aluminium on the transport of hydrogen and on the increase of hydrogen corrosion resistance of Ti, Ni, and Fe.
4. Determination of correction factors connected with the quantitative analysis by electron spectroscopies (*e.g.* the backscattering factor in Auger electron spectroscopy and the active cross-section for the elastic scattering of electrons).
5. Application of simulation methods of the electron transport theory in solids for the analysis of the effects of elastic and non-elastic electron scattering on the surface of solids. Determination of a value of the inelastic mean free path, material coefficients in Chen's and Werber's rules for the estimation of a correction parameter for non-elastic losses of an electron in chosen elements and alloys. Determination of thickness of layers and the mechanism of the layer growth and investigation of interlayer surface for the overlayer substrate system.
6. Investigation with the use of Monte-Carlo method of dependence of the elastic peak intensity on the thickness of metal overlayers on various substrates.
7. New models for equation of state with association for phase equilibria determinations.

The Department includes the Center for Physical Chemistry of Materials which carries out work on the following issues:

1. Electrochemical and corrosion properties of amorphous materials and their components.
2. Identification and role of local phenomena in the whole electrode process. Significance of local phenomena in electrocatalysis and local corrosion.
3. Dynamics of electrocatalytic and corrosion processes. Influence of passivation and inhibition of electrode processes on the creation of unstability and surface structures.
4. Surface diffusion and surface reactions in electrocatalytic processes on metallic electrodes.

The Department is a coordinator and principal contractor of the Centre of Excellence "Surface Phenomena and Reactions" (SURPHARE) in the framework of the European Union Programme "Competitive and Sustainable Growth Research Programme" (2002–2005).

Tadeusz Zakroczymski, Professor

M.Sc., 1968 – Department of Chemistry, Technical University of Warsaw
Ph.D., 1976 – Institute of Physical Chemistry, Warsaw
D.Sc., 1992 – Institute of Physical Chemistry, Warsaw
Professor, 2004 – Institute of Pfysical Chemistry, Warsaw

Education and training:

1976–77 – University of Newcastle upon Tyne, Great Britain
1984–85 – Ohio State University, Columbus, USA

Research areas:

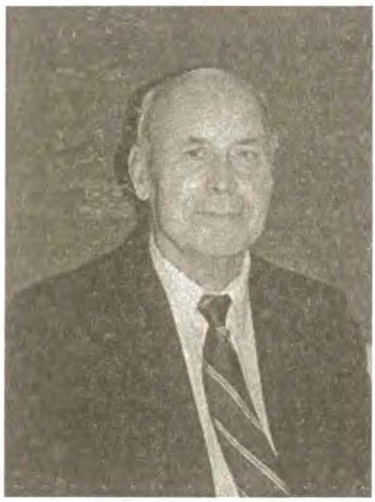
- Entry, transport, absorption, and trapping of hydrogen in metals
- Electrochemistry and corrosion of metals
- Surface modifications of metals

Selected papers

1. Zakroczymski T., "Entry of Hydrogen into Iron Alloys from the Liquid Phase"; in "Hydrogen Degradation of Ferrous Alloys" (R.A. Oriani, J.P. Hirth, M. Śmiałowski, Eds.) Noyes Publications, Park Ridge, New Jersey, U.S.A., (1985).
2. Zakroczymski T., Łukomski N. and Flis J., "Entry and Transport of Hydrogen in Ion Nitrided Iron", *J. Electrochem. Soc.*, **140**, 3578 (1993).
3. Zakroczymski T., Łukomski N. and Flis J., "Effect of Plasma Nitriding-Base Treatments on the Absorption of Hydrogen by Iron", *Corr. Sci.*, **37**, 811 (1995).
4. Zakroczymski T. and Flis J., "Impedance Characterization of the Activation of Iron Surface for Hydrogen Entry from Alkaline Solution", *Electrochim. Acta*, **41**, 1245 (1996).
5. Zakroczymski T., Kleshnya V. and Flis J., „Evolution and Entry of Hydrogen into Iron during Cathodic Charging in Alkaline Solution with Ethylenediaminetetraacetic Acid", *J. Electrochem. Soc.*, **145**, 1142–1148 (1998).
6. Zakroczymski T., "Electrochemical Determination of Hydrogen in Metals", J. *Electroanal. Chem.*, **475**, 82–88 (1999).
7. Owczarek E. and Zakroczymski T., "Hydrogen Transport in a Duplex Stainless Steel", *Acta Mater.*, **48**, 3059–3070 (2000).
8. Zakroczymski T., Flis J., Łukomski N. and Mańkowski J., "Entry, transport and absorption of hydrogen in low-temperature plasma nitrided austenitic stainless steel", *Acta Mater.*, **49**, 1929–1938 (2001).
9. Zakroczymski T. and Owczarek E. "Electrochemical Investigation of Hydrogen Absorption in a Duplex Stainless Steel", *Acta mater.*, **50**, 2701–2713 (2002).
10. Wolarek Z. and Zakroczymski T., "Hydrogen Transport in Plasma Nitrided Iron", *Acta mater.*, **52**, 2637–2643 (2004).

Total number of publications: 115

Janusz Flis, Professor Emeritus



M.Sc., 1956 – Department of Chemistry, Technical University of Warsaw
Ph.D., 1964 – Institute of Physical Chemistry, Warsaw
D.Sc., 1975 – Institute of Physical Chemistry, Warsaw
Professor, 1991 – Institute of Physical Chemistry, Warsaw

Education and training:

1965–66 – Leeds University, Great Britain
1980–81 – Rensselaer Polytechnic Institute, Troy, USA
1986 – CNRS, Université P. et M. Curie, Paris, France
1990–91 – Pennsylvania State University, State College, USA
1995 – Kawasaki Steel Corporation, Technical Research Laboratories, Chiba, Japan

Editorial affiliation:

- Associate editor of "*Corrosion Protection*" (Polish monthly).

Research areas:

- Electrochemistry and corrosion of metals
- Localised corrosion
- Passivation and inhibition
- Hydrogen in metals
- Surface modification
- Protective coatings

Selected papers

1. Flis J. and Sikora E., "Impedance and transient study of iron and iron-phosphorus alloy in carbonate/bicarbonate solution with phosphate ions", *Electrochim. Acta*, **39**, 1145–1149 (1994).
2. Odziemkowski M., Flis J. and Irish D.E., "Raman spectral and electrochemical studies of surface film formation on iron and its alloys with carbon in $Na_2CO_3/NaHCO_3$ solutions with reference to stress corrosion cracking", *Electrochim. Acta*, **39**, 2225–2236 (1994).
3. Flis J. and Wiliński J., "The use of rotating split-ring disc electrode for the estimation of Fe(II) and Fe(III) species in surface layers on iron in borate buffer, *Materials Science Forum*, **185–188**, 641–648 (1995).
4. Flis J. and Zakroczymski T., "Impedance study of reinforcing steel in simulated pore solution with tannin", *J. Electrochem. Soc.*, **143**, 2458–2464 (1996).
5. Flis J., Pickering H.W. and Osseo-Asare K., "Interpretation of impedance data for reinforcing steel in alkaline solution containing chlorides and acetates", *Electrochim. Acta*, **43**, 1921–1929 (1998).
6. Flis J., Mańkowski J., Zakroczymski T. and Bell T., "The formation of phosphate coatings on nitrided stainless steel", *Corros. Sci.*, **43**, 1711–1725 (2001).
7. Zakroczymski T., Flis J., Lukomski N. and Mańkowski J., "Entry, transport and absorption of hydrogen in low-temperature plasma nitrided austenitic stainless steel", *Acta mater.*, **49**, 1929–1938 (2001).

Total number of publications: 122

Aleksander Jabłoński, Profesor

M.Sc., 1969 – Department of Chemical Technology, Technical University of Szczecin

Ph.D., 1975 – Institute of Physical Chemistry, Warsaw

D.Sc., 1982 – Institute of Physical Chemistry, Warsaw

Professor, 1990 – Institute of Physical Chemistry, Warsaw

Education and training:

1975–76 Department of Chemistry, University of California, Berkeley, USA

1983–84 Institute of Physical Chemistry, University of Munich, Germany (Humboldt Foundation Fellow)

1990 – Institute of Inorganic and Theoretical Chemistry, University of Bonn, Germany (Humboldt Foundation Fellow)

1992 – Research Institute of Electronics, Shizuoka University, Hamamatsu, Japan (Visiting Professor)

1993 – Institut of Technical and Applied Physics, Technical University of Vienna, Austria (Visiting Professor)

1996 – Institute of Physics, University of Odense, Denmark (Visiting Professor)

Professional affiliations:

- Polish Vacuum Society
- International Union for Vacuum Science, Technique and Applications (IUVSTA), Applied
- Surface Science Division
- Surface Analysis Society of Japan

Research areas:

- Studies of solids by surface sensitive electron spectroscopies: x-ray photoelectron spectroscopy and Auger electron spectroscopy
- Theory of electron transport in solids, theoretical analysis of interaction: electron – solid surface
- Qualitative and quantitative analysis of solid surfaces

Selected papers

1. Jabłoński A., "Transport Cross Section for Electrons at Energies of Surface-Sensitive Spectroscopies", *Phys. Rev.*, **B58**, 16470 (1998).
2. Dubus A., Jabłoński A. and Tougaard S., "Evaluation of Theoretical Models of Elastic Electron Backscattering from Surfaces", *Progress in Surface Science*, **63**, 135 (2000).
3. Jabłoński A., Determination of the IMFP from Electron Elastic Backscattering Probability", *Surface Interface Anal.*, **29**, 582 (2000).
4. Jabłoński A., "Remarks on the Definition of the Backscattering Factor in AES", *Surface Sci.*, **499**, 219 (2002).
5. Jabłoński A. and Powell C.J., "The Electron Attenuation Length Revisited", *Surface Science Reports*, **47**, 33 (2002).
6. Jabłoński A., "Analytical Applications of Elastic Electron Backscattering from Surfaces ", *Progress Surface Sci.*, **74**, 357 (2003).
7. Jabłoński A., Salvat F. and Powell C.J., "Comparison of Electron Elastic-Scattering Cross Section Calculated from Two Commonly Used Atomic Potentials", *J. Phys. Chem. Ref. Data*, **33**, 409 (2004).

Total number of publications: 220

Maria Janik-Czachor, Professor

M.Sc., 1963 – Department of Chemistry, Technical University of Warsaw
Ph.D., 1968 – Institute of Physical Chemistry, Warsaw
D.Sc., 1984 – Institute of Physical Chemistry, Warsaw
Professor, 2003 – Institute of Physical Chemistry, Warsaw

Education and training:

1974–75 – Alexander von Humboldt Fellow, Max Planck Institut für Eisenforschung, Dusseldorf, Germany
1980 – Visiting Research Fellow at Chemistry Dept., Northwestern University, Evanston, USA and Consultant there (several times during 1981–85)
1983 – Consultant, Corrosion Research Centre, University of Minnesota, Minneapolis, USA
1986 – Alexander von Humboldt Fellow, Max Planck Institut für Eisenforschung, Dusseldorf, Germany
1989 – Japanese Society for Promotion of Science Fellow, Visiting Professor, Tohoku University, Sendai, Japan
1996 – Visiting Professor, University of Geneve, Switzerland
2000 – Visiting Professor, Institute National Politechnique de Toulouse, Toulouse, France

Professional affiliations:

- International Society of Electrochemistry (ISE)
- Polish Chemical Society

Research areas:

- Corrosion and degradation of metals
- Passivity and stability of the passive state of metals and alloys
- Surface analysis (electron and optical spectroscopies)
- Reactivity of novel materials

Selected papers

1. Wołowik A., Janik-Czachor M. and Szummer A., "Breakdown of Passivity of Al.-refractory Metal Amorphus Alloys", *Proc. Symp. on Passivity and its Breakdown* (Eds. P.M. Natishan, H.S. Isaacs, M. Janik-Czachor, V.A. Macagno, P. Marcus, M. Seo) Pennington 1998, pp. 533–543.
2. Janik-Czachor M., Kudelski A., Dolata M., Varga M., Szummer A., Bukowska J. and Molnár Á., "Modification of Surface Activity of Cu-Zr Amorphous Alloys and Cu Metal by Electrochemical Methods", *Mat. Sci. Eng. A-Struct.*, **267**, (2)235–239, 1999.
3. Janik-Czachor M., Szummer A., Molnár Á., Dolata M., Kudelski A. Varga M., Bukowska J. and Sikorski K., "Electrochemical Modification of Cu-Zr Amorphous Alloys for Catalysis", *Electrochim. Acta,* **45**, 3295 (2000).
4. Szummer A., Janik-Czachor M., Molnár Á., Marchuk I., Varga M. and Filipek S.M., "Effect of Hydrogenation under high Pressure on the Structure and Catalytic Properties of CuZr Amorphous Alloys", *Journal of Molecular Catalysis A: Chemical*, Volume: **176**, Issue: 1–2, November 20, pp. 205–212 (2001).
5. Janik-Czachor M., Jaśkiewicz A., Kędzierzawski P. and Werner Z., "Stability of the passive state of Al-Ta and Al-Nb amorphous alloys", *Mat. Sci. Eng. A*, **358** (2003) 171–177.
6. Janik-Czachor M., Bukowska J. Szummer A., Molnar A., Mack P., Filipek S.M., Kędzierzawski P., Kudelski A., Pisarek M., Dolata M. and Varga M., "Modification of Surface Activity of Cu-based Amorphous Alloys by Chemical Processes of Metal Degradation", *Aplied Catalysis A*, **235**, 157–169 (2002), and *ibid*, **253**, 539–541 (2003).

Total number of publications: 120

Ellina Łunarska, Professor

Professor, Department of Electrochemistry and Corrosion, Institute of Physical Chemistry of the Polish Academy of Science, Warsaw, Poland,

Professor, Faculty of Mathematics and Natural Sciences, Cardinal Stefan Wyszynski University Warsaw, Poland

Education and traning:

M.Sc., – in material sciences, 1960, Technical University, Kharkov, USSR

Ph.D., – in Physical Chemistry, 1972, Institute of Physical Chemistry, Warsaw, Poland

D.Sc., – in Physical Metallurgy, 1984, Academy of Mining and Metallurgy, Krakow, Poland

1979/80 – University of Notre Dame, Notre Dame USA

1985/86 – Ohio State University, Columbus, USA

1997 – University of Jaen, Andalusia, Spain

2000 – US Energy Department, Albany Research Center, Albany, Oregon USA

Research areas:

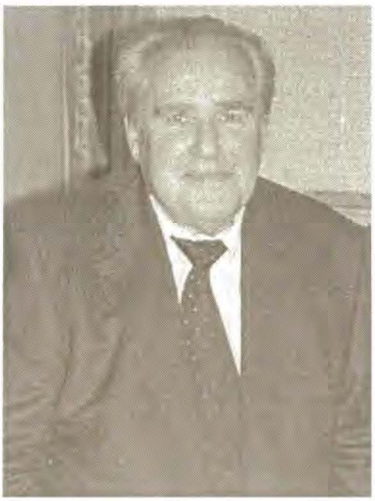
- Hydrogen effects on elastic and plastic properties of metals
- Surface modification for corrosion and hydrogen uptake protection
- Stress corrosion cracking of metals and alloys
- Hydrogen assisted corrosion of industrial installations

Selected papers

1. Łunarska E., "Effect of hydrogen on the plastic properties of iron single crystalss, whiskers and polycrystals", "Hydrogen Degradation Effects in Iron Base Alloys" J.P. Hirth, R.A. Oriani, M. Śmiałowski, eds., Noyes Publ., New Jersej, p. 321 (1985).
2. Łunarska E., "Hydrogen-induced degradation of carbon steels", in "Hydrogen Degradation Effects in Iron Base Alloys" J.P. Hirth, R.A. Oriani,M. Śmiałowski, eds., Noyes Publ. New Jersey, p. 712 (1985,).
3. Łunarska E. and Zieliński A., "Anelasticity", "Hydrogen Degradation Effects in Iron Base Alloys" R.A. Oriani, J.P. Hirth, M. Śmiałowski, eds., Noyes Publ., New Jersey, p. 289 (1985,).
4. Łunarska E.,"Hydrogen behavior in the iron surface layer modified by plasma nitriding and ion boronising" Materials and Corrosion, **51**, 1–9, (2000).
5. Łunarska E. and Samatowicz D.,"The hydrogen-induced modification of the properties of the surface coated with oil and lubricant" "Tribology Intern., **33**, 491–499, (2000).
6. Łunarska E. and Zaborski St., "Hydrogen effects in anodic grinding of Ti alloy", Wear, **249**, 606–616, (2001).
7. Łunarska E., Ziomek-Moroz M. and Michalski A., "Electrochemical determination of penetrating porosity and the chemical and phase composition of pulse plasma deposited Ti-Al and Ni-Al coatings", Intermetallics, **9**, 711–719, 2001, p. 289 (1985,).
8. Łunarska E., Nikifirow K., Wierzchoń T. and Ulbin-Pokorska I., "Effect of plasma nitriding on hydrogen behavior in electroplated chromium coating", Surface and Coating Technology, **145**, 139–145 (2001).
9. Łunarska E., Czerniajewa O. and Nakonieczny A., "Effect of plasma nitriding and TiN plasma deposition on stress corrosion cracking of 40HM steel", Vacuum, **63**, 469–473 (2001).
10. Łunarska E., Nikifirow K. and Sitko E., "Stress corrosion cracking of bainite 0.2C-1Cr-1Mn-1Si-1Mi type steel in acid rain simulated solution", Materials and Corrosion, **55**, 156–168 (2004).

Total number of publication: 156

Andrzej Mączyński, Associate Professor



M.Sc., 1955 – Department of Chemistry, Warsaw University
Ph.D., 1963 – Institute of Physical Chemistry, Warsaw

Professional affiliations:

- CODATA – Committee on Data for Science and Technology, (pass Task Group Chairman; Member of the Polish National CODATA Committee)
- IUPAC – International Union on Pure and Applied Chemistry (pass Member the Commission on Solubility Data; Member of the Subcommittee on Liquid-Liquid Solubility; Member of the Editorial Board of the Solubility Data Series)
- "International Data Series, Selected Data on Mixtures" (K. Marsh, Ed.); Thermodynamics Research Center, Texas A&M University, Texas, USA, (Executive Director, 1993–2000)
- "International Data Series, Selected Data on Mixtures" (J. Rainwater, Ed.); Thermodynamics Research Center, National Institute of Standards and Technology, Boulder, (Associate Editor, since 2000)
- "Vapor-Liquid Equilibria, Series", Thermodynamics Data Center, Warsaw, (Editor-in-Chief, since 1997)

Research areas:

- Thermodynamics
- Collection, correlation, critical evaluation, and prediction of phase equilibrium data

Selected papers

1. "Thermodynamics Data For Technology", (A. Bylicki, Ed.), PWN, Warszwa, Vols 1– 0 (1976–1988);
2. "IUPAC Solubility Data Series", Pergamon Press, Oxford, New York, Tokyo, Vols 15, 30, 37, 38, 48, 49 and 56 (1984–1994).
3. "IUPAC Solubility Data Series", (Skrzecz A., Shaw and S. Mączyński A., Eds), Vol. 69, Journal of Physical and Chemical Reference Data, Vol. 69 (1999).
4. "International Data Series – Selected Data on Mixtures" (Marsh K., Ed.); Thermodynamics Research Center, Texas A&M University, Texas, USA, Vols 22–28, (1993–2000).
5. "International Data Series – Selected Data on Mixtures" (Rainwater J., Ed.); Thermodynamics Research Center, National Institute of Standards and Technology, Boulder, Co, USA, Vols 29-32, (2002–2004).
6. "Vapor-Liquid Equilibria, Series", (Mączyński A., Ed.), Thermodynamics Data Cener, Warszawa, Vols 1–12 (1997–2001).
7. Mączyński A., Goral M., Wiśniewska-Goclowska B., Skrzecz A. and Shaw D., "Monatshefte für Chemie" **134**, 633 (2003).
8. Recommended Vapor-Liquid Equilibrium Data, Parts 1–3, Journal of Physical and Chemical Reference Data (2002–2004).
9. Recommended Liquid-Liquid Equilibrium Data, Parts 1–3, Journal of Physical and Chemical Reference Data (2004).
10. "IUPAC-NIST Solubility Data Series" (Mączyński A. and Shaw D., Eds), Vol. 81, Parts 1–12, Journal of Physical and Chemical Reference Data, in press.

Marian Góral, Research Associate

M.Sc., 1970 – Department of Chemistry, University of Warsaw

Ph.D., 1975 – Department of Chemistry, University of Warsaw

D.Sc., 2004 – Department of Chemistry, University of Warsaw

Education and training:

1979–1980 University Erlangen Nuerenberg

1985–1986 University Erlangen Nuerenberg

Research areas:

Phase Equilibria in associated binary and multicomponent mixtures.

- Modelling of associating systems.
- Correlation and prediction of mutual solubilities in systems of water/sea water + organic solvents.
- Prediction of vapor–liquid equilibria in associating systems.
- High pressure vapor–liquid equilibria.
- Preparation of recommended data and software for industry.

Selected papers

1. Góral M., "Correlation of VLE in associating mixtures with cubic equation of state". *Fluid Phase Equilibria*, **118**, 27 59 (1996).
2. Góral M., Oracz P. and Warycha S., "Vapour–liquid equilibria XI. The quaternary system cyclohexane+hexane+acetone+ methanol at 313.15 K". *Fluid Phase Equilibria*, **135**, 51–61 (1997).
3. Góral M., "Correlation, verification and prediction of vapour-liquid equilibria using equation of state with association term I. Alcohols + aliphatic hydrocarbons", *Fluid Phase Equilibria*, **178**, 149–167 (2001).
4. Góral M., "Correlation, verification and prediction of vapour-liquid equilibria using equation of state with association term II. Alcohols + non–aliphatic hydrocarbons", *Fluid Phase Equilibria*, **193**, 97–107 (2002).
5. Maczynski A., Góral M., Goclowska B.W., Skrzecz A. ans Shaw D., "Mutual solubilities of water and hydrocarbons". *Monatshefte fuer Chemie/Chemical Monthly*. **134**, 633 (2003).
6. Mączyński A., Wiśniewska-Gocłowska B. and Góral M., "Recommended Liquid-Liquid Equilibrium Data, Part 1: Binary C5–C11 Alkane – Water Systems", *J. Phys. Chem. Ref. Data*, **33**, 549 (2004).
7. Góral M., Mączyński A. and Wiśniewska-Gocłowska B., "Recommended Liquid-Liquid Equilibrium Data, Part 2: Unsaturated Hydrocarbon – Water Systems". *J. Phys. Chem. Ref. Data*, **33**, 579 (2004).
8. Góral M., Oracz P., Skrzecz A., Bok A. and Mączyński A., "Recommended Vapor-Liquid Equilibrium Data. Part 3. Binary Alkanol – Aromatic Hydrocarbon Systems", *J. Phys. Chem. Ref. Data*, **33**, 959 (2004).

Total number of publications: 54

Beata Lesiak-Orłowska, Research Associate

M.Sc., 1983 – Department of Physics University of Warsaw, Warszawa, Poland
Ph.D., 1991 – Institute of Physics Polish Academy of Sciences, Warszawa, Poland
D.Sc., 2004 – Department of Physics and Astronomy University of Wrocław, Wrocław, Poland

Education and training:

1992/1993 – post doctorate scholarship of the Royal Society, Department of Chemistry University of Cambridge, Cambridge, UK

co-operations:

- Institute of Biocybernetics and Biomedical Engineering Polish Academy of Sciences, Warszawa, Poland
- Institute of Physics Academy of Sciences of the Czech Republic, Prague, Czech Republic
- Research Institute of Technical Physics and Material Sciences Hungarian Academy of Sciences, Budapest, Hungary
- Research Institute of Nuclear Physics Hungarian Academy of Sciences, Debrecen, Hungary
- DESSY Synchrotron Laboratory, Hamburg, Germany
- University of Strasbourg, Strasbourg, France

Research areas:

– quantitative and qualitative analysis by Auger electron spectroscopy (AES) and x-ray photoelectron spectroscopy (XPS) of complex systems, *e.g.* multicomponent samples, polymers, overlayers on substrates
– applications of pattern recognition methods for electron spectroscopy methods (XPS and AES) for qualitative and quantitative analyses
– investigating the electron elastic backscattering coefficient; application of elastic peak electron spectroscopy (EPES) for determining the electron transport parameter, *i.e.* the inelastic mean free path (IMFP) using the Monte Carlo model of electron transport in a solid
– determining of electron inelastic losses using the EPES method
– application of the EPES method for qualitative and quantitative analysis

Selected papers

1. Hoogers G., Lesiak-Orłowska B. and King D. A., "Diffusion on a stepped surfaces: H and D on Rh{332}", *Surf. Sci.*, **327**, 47–52 (1995).
2. Lesiak B., Zemek J. and Jóźwik A., "Phase distinction in semi-insulating polycrystalline silicon by pattern recognition of XPS/XAES data", *Appl. Surf. Sci.*, **135**, 318–330 (1998).
3. Lesiak B., Jablonski A., Zemek J. Trchova M. and Stejskal J., "Characterisation of polyaniline and determination of the inelastic mean free path of electrons by elastic peak electron spectroscopy", *Langmuir*, **16**, 1415–1423 (2000).
4. Varga D., Kövér L., Tóth J., Tokesi K., Lesiak B., Jablonski A., Robert C., Gruzza B. and Bideux L., "Determination of yield ratios of elastically backscattered electrons for deriving inelastic mean free paths in solid", *Surf. Interface Anal.*, **30**, 202–206 (2000).
5. Sulyok A., Gergely G., Menyhard M., Tóth J., Varga D., Kövér L., Berenyi Z., Lesiak B. and Kosiński A., "Recoil effect in carbon structures and in polymers", *Vacuum*, **63**, 371–376 (2001).
6. Jiricek P., Zemek J., Lejcek P., Lesiak B., Jablonski A. and Cernanský M., "Stability of the inelastic mean free paths determined by elastic peak electron spectroscopy in nickel and silicon", *J. Vac. Sci. Technol.*, **A20**, 447–455 (2002).
7. Kövér L., Tóth J., Varga D., Lesiak B. and Jablonski A., "Surface composition of alloys derived from elastic peak intensity", *Surf. Sci.*, **507–510**, 895-899 (2002).
8. Zemek J., Jiricek P., Jablonski A. and Lesiak B., "Growth mode and morphology of ultrathin gold films deposited on nickel", *Appl. Surf. Sci.*, **199**, 138–147 (2002).
9. Orosz G. T., Gergely G., Menyhard M., Tóth J., Varga D., Lesiak B. and Jablonski A., "Hydrogen and surface excitation in electron spectra of polyaniline", *Surf. Sci.*, **566–568**, 544–548 (2004).

Total number of publications: 68

Laboratory of Electrochemistry and Surface Analysis in Corrosion Studies

Head: Prof. Janusz Flis

The Laboratory offers scientific service in the form of research studies or measurements in the field of electrochemistry and surface analysis, associated with corrosion processes on metals and on their modified surfaces. The research involves the areas as follows:

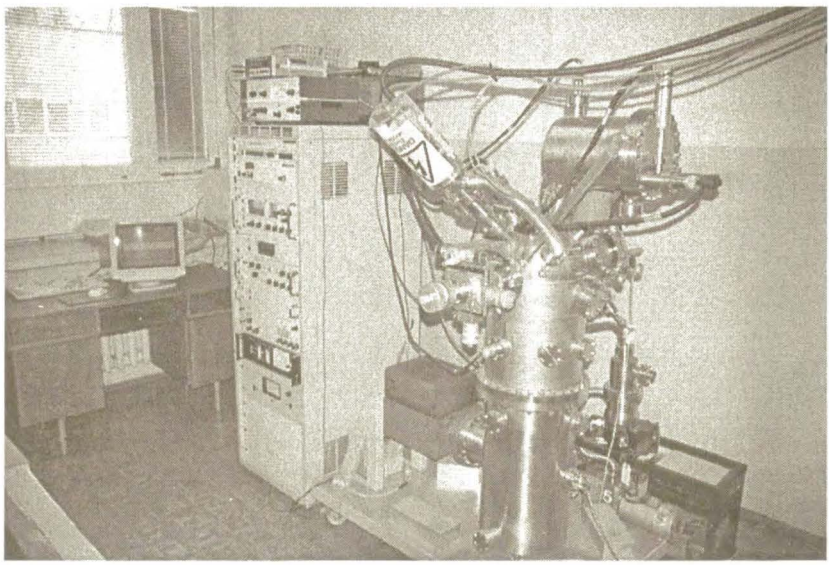
Corrosion behaviour and passivation of metals and modified surfaces
- determination of corrosion rate by electrochemical methods
- examination of the growth of passive films by ellipsometry and AES/XPS
- study of localised corrosion and inhibition
- modification of the metal surface by PA CVD and by chemical methods

Effect of hydrogen on mechanical properties of metals and its interaction with structural defects
- determination of the content of hydrogen in materials from exploited equipment
- predicting the lifetime of an equipment with a given content of hydrogen
- study of hydrogen embrittlement
- study of interaction of hydrogen with defects in metals
- diffusion, absorption and trapping of hydrogen in metals

Analysis of surface films by AES and XPS
- determination of the elemental concentration-depth profiles in surface layers
- analysis of protective layers obtained by chemical and electrochemical treatments

Equipment

Electrochemical measurements
- facilities for *dc* and *ac* (EIS) measurements
  - Solartron FRA 1255 and EI 1286
  - Gamry Instruments CMS100 System, including CMS105 DC Corrosion Measurement System, CMS130 Cyclic Voltammetry, and CMS300 Electrochemical Impedance System



- cells for the electrochemical determination of hydrogen permeation and absorption
- a system for fast transient measurements
- rotating disc electrodes and a rotating disc with split-ring electrode

Surface analysis
- electron spectrometer AES and XPS
- automatic ellipsometer

Hydrogen in metals
- determination of hydrogen content by vacuum extraction
- determination of the mobile an reversibly trapped hydrogen by the electrochemical technique

Surface modification
- installation for PA CVD

Mechanical testing
- Instron Testing Machine
- a machine for high range of strain rates

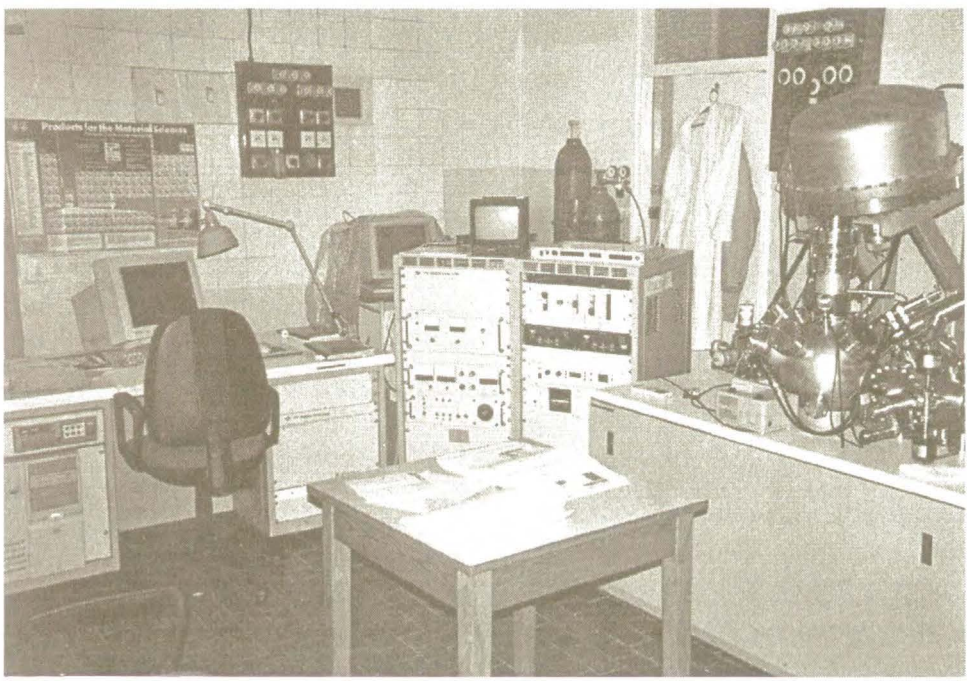
Contact persons:

Prof. Janusz Flis; jflis@ichf.edu.pl;
Affiliation: Department of Electrochemistry and Corrosion
tel.: +(22) 343-3235

Laboratory of Electron Spectroscopies (AES-XPS) for Studies of Solid Surfaces

Head: Prof. Aleksander Jabłoński

Numerous branches of technology and science (catalysis, corrosion science, microelectronics, etc) frequently require information about chemical state and the composition of the surface layer of thickness in the nanometer range. Such thicknesses are comparable with first several atomic layers. This information can be obtained with the use of surface sensitive electron spectroscopies: x-ray photoelectron spectroscopy and Auger electron spectroscopy.



Equipment

In Laboratory of Electron Spectroscopy, two spectrometers are installed:

- Photoelectron spectrometer ESCALAB-210 produced by VG Scientific equipped with preparation chamber. The preparation chamber makes possible preparation of a samples to analysis: annealing in the temperature range from –80° C to 800°C, and interaction with different gases. The sample transmission system makes possible fast introduction of samples to the main chamber of the spectrometer. This spectrometer is controlled by the computer with the installed software packet ECLIPSE.
- Auger electron spectrometer based on the electron energy analyser DCMA produced by Physical Electronics. The analysed electron energies range from 50 eV to 2000 eV, and the energy resolution of this analyser is 0.6% of the anlysed energy. The vacuum system and the system for data acquision and processing is of Polish design and production (OBREP, Technical University of Warsaw).

Data processing

The following information can be derived from the recorded spectra using the currently available software:

- Identification of elements present in the surface layer submitted to analysis
- Chemical state of elements. In selected cases, it is possible to identify compounds.
- Determination of surface composition

From the shape of the recorded spectra, it is also possible to identify the structure of the surface region using the software packet QUASES (overlayer thickness, presence of islands, in-depth concentration profile, *etc.*).

Contact person:

Dr. Janusz W. Sobczak; jws@ichf.edu.pl

Center for Physical Chemistry of Materials
(Institute of Physical Chemistry PAS and Faculty of Material Science WUT)

Head: Prof. Maria Janik-Czachor

Tel.: (0 22) 343-3325; Fax: (0 22) 6325276
e-mail: maria@ichf.edu.pl

Topics:

1. Electrochemical and corrosion properties of metallic glasses and their components, 2. Dynamics of electrocatalytic processes, 3. Local phenomena at electrodes, 4. High resolution characterization of nonhomogeneous functional and construction materials.

- ***High resolution morphological and microchemical analysis (SEM and SAM)***

Characterization of surfaces of new materials including nanomaterials is an important task for both chemists and material scientists interested in understanding and improving their performance as functional and/or contruction materials. The most suitable techniques for such analysis are Scanning Auger Microanalysis (SAM) combined with Scanning Electron Microscopy (SEM). Chemical analysis of a selected nano-area or a thin surface film can be performed with the aid of a Scanning Auger Microprobe.

Apparatus

The Physical Chemistry of Materials Center is equipped with a Microlab 350 (Thermo VG Scientific, UK) which is a high resolution Auger system also capable of performing multi-technique analysis and with the option of being fitted with a range of preparation facilities. Its key features are:

- Spatial resolution: 7 nm SEM-Scanning Electron Microscopy, 12 nm SAM-Scanning Auger Microscopy
- High sensitivity
- User selectable energy resolution 0.6% – 0.06%
- Multi-technique capability (AES-Auger Electron Spectroscopy, XPS-X-ray Photoelectron Spectroscopy)
- *Avantage*, a Windows based data system

Microlab 350 is a high-performance scanning Auger instrument using field emission technology to provide high spatial resolution. The spherical sector analyzer (SSA), used on the Microlab 350, allows analysts to select the best combination of energy resolution and sensitivity for each analysis, in common with most other spectroscopic techniques. The Microlab 350 additionally is equipped with:

* an X-ray gun (twin anode source: AlK_α, MgK_α) for XPS measurements (spatial distribution: average value from all sample surface area); this extends the use of this instrument to dielectric materials,
* an ion gun for sputter etching; the ion gun is usually used for depth profiling, sample cleaning and charge compensation.

This instrument is particularly useful in investigating small surface features, thin layers, impurities in materials as well as in determining their chemical (elemental) composition and chemical state of their components.

Sample preparation for surface analysis

Samples cannot exceed 10×10 mm surface area and 10 mm thickness. AES technique is limited to conducting materials: metals and semiconductors of sufficient conductivity. The stability of samples in ultra-high vacuum conditions is required (pressure lower than 10^{-10} mb).

Restrains

Samples containing elements such as Hg, Te, Cs, K, Na, As, J, Zn, Se, P, S, *etc.* or their compounds cannot be analysed because of the possibility of damage to the analyser. The same concerns samples which decompose with emission of compounds such as H_2O, HCl and H_2S under conditions of ultra-high vacuum and/or X-ray radiation.

Local chemical analysis

The following surface information can be obtained:

1. Chemical composition maps of the surface with nano-scale resolution [M.Janik-Czachor, J.Bukowska, A.Szummer, A.Molnar, P.Mack, S.M.Filipek, P.Kędzierzawski, A.Kudelski, M.Pisarek, M.Dolata, M.Varga: Modification of Surface Activity of Cu-based Amorphous Alloys by Chemical Processes of Metal Degradation, *Applied Catalysis A*, **235** (2002) 157 and **253**, 539 (2003), A. Szummer, M. Janik-Czachor, P. Mack, M. Pisarek: High resolution electron probe characterization of modified Cu-based amorphous alloys, *Microscopy & Microanalysis*, Vol. **9**, 359 (2003).

2. Local information on surface composition and on the chemical state of surface components in nano areas [Catalytic Activity of Cu-Based Amorphous Alloy Ribbons Modified by Cathodic Hydrogen Charging by M. Pisarek, M. Janik-Czachor, A. Molnar and K. Hughes, *Appl. Catal. A*, **283**,177 (2005).

3. Composition profiles of thin surface films with a depth resolution below a nm [M. Janik-Czachor, A. Jaskiewicz, M. Dolata, Z.Werner, Passivity and its breakdown in Al-based amorphous alloys, *Materials Chemistry and Physics*, in press 2005)].

- ***Scanning Electrochemical Microscopy***

The Scanning Electrochemical Microscope designed by dr M. Dolata and dr P. Kędzierzawski and built in the Institute of Physical Chemistry PAS is a scanning probe instrument, which makes is possible to measure the distribution of quantities such as potential, current or pH over a surface of metal or semiconductor electrode. The instrument consists of an X-Y stage propelled by stepper motors and used to move a microsensor near the surface of the electrode, a motor controller, a potentiostat, a low noise and high input impedance signal conditioning system and a data acquisition system. Both movement of the microsensor and measurements are computer-controlled with a program developed at the Institute. The Microscope has a step size of 0.3 μm and lateral resolution of the order of μms depending on sensor size, distance from the electrode and electrode roughness.

Application areas

Local corrosion studies, galvanic and paint coatings studies, corrosion and electrocatalysis studies of composite materials, electrode mechanisms, microstructure deposition using Scanning Counter Electrode technique.

Sample limitations

The instrument will accommodate plain samples of conducting material of a diameter of 8 mm and a height of 10 mm.

- ***Electrochemical System for Corrosion Studies***

The system consists of an EP-20 potentiostat and an EG-20 function generator from ELPAN, data acquisition system from Ambex, Poland and a selection of electrochemical cells adapted for various types of measurements. The measurements are controlled with programs developed at the Institute.

Application areas

Electrochemical corrosion studies: determination of corrosion rate, polarization curves, local corrosion studies, electrode mechanism studies.

Consultants:

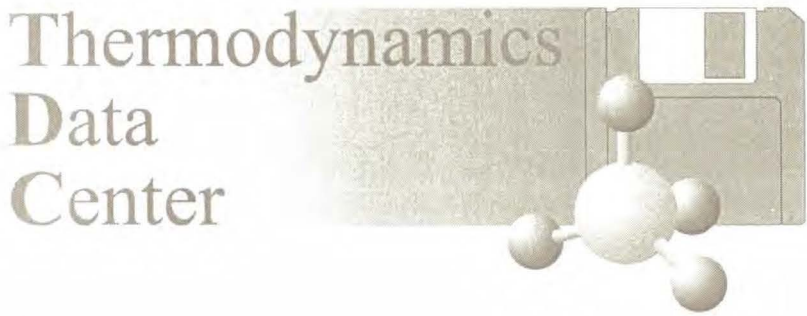
Prof. A. Szummer, Prof. K. Sikorski, Prof. Z. Werner

Information available:

Department of Electrochemistry, Corrosion and Applied Surface Science
Institute of Physical Chemistry, Polish Academy of Sciences
Kasprzaka 44/52, 01-224 Warszawa
tel.: +48 (22) 343-3325, fax: +48 (22) 6325276
e-mail: maria@ichf.edu.pl or marcinp@ichf.edu.pl

Thermodynamics Data Center

Head: Dr. Adam Skrzecz



The TDC – Thermodynamics Data Center has been created by the following partners:

- Institute of Physical Chemistry, Polish Academy of Sciences
- Institute of Coal Chemistry, Polish Academy of Sciences
- Faculty of Chemistry, Warsaw University
- Faculty of Chemistry, Warsaw University of Technology

The TDC closely cooperates with:

- The Wojciech Swiętosławski Foundation for the Promotion and Development of Science in Poland
- TRC-NIST – Thermodynamics Research Center, National Institute of Standards and Technology, Boulder, Co, USA

An essential part of the activity of the TDC are methods of critical evaluation, correlation and prediction of thermodynamics data, mainly vapor-liquid and liquid-liquid equilibrium data. Critical evaluation of data are based mainly on regressions, thermodynamic consistency tests, and mutual correlations of thermodynamics functions.
Correlations of date are based mainly on the following equations: Redlich-Kister, Van Ness-Van Laar, Wilson, NRTL, UNIQAC, Peng-Robinson, and Redlich-Kwong.
Predictions of data are based mainly on the UNIFAC method and Equations of State with an association therm.

All these methods, programs, and collected and evaluated data are applied for publication series, papers, CD ROMs, and special reports.

Publication Series

1. Vapor – Liquid Equilibria Series.
   Each volume of this Series contains selected VLE data for a particular group of binary systems. All the data have been correlated by a chosen equation, mainly Wilson, NRTL or Goral EoS. Since 1998 eleven volumes of this series have been published by the TDC. They are also available on CD ROM.
2. IUPAC Solubility Data Series
   Each volume of this Series contains experimental liquid-liquid equilibrium and solubility data with critical evaluations and recommendations for particular systems. Since 1979 seventy three volumes of this series have been published by the Pergamon Press, Oxford Press and receantly by the Journal of Physical and Chemical Reference Data. Since 1984 nine volumes of this Series have been prepared in the cooperation with the Institute of Physical Chemistry PAS.

3. International Data Series – Selected Data on Mixtures.
   The International Data Series contains selected and calculated VLE, LLE, SLE, H^E, and V^E data for binary mixtures at moderate pressure. Since 1973 four issues per year were published by TRC - Texas A&M University until 2000 and next by the TRC - National Institute of Standards and Technology, USA. Since 1993 thirty four issues were prepared in the cooperation with the TDC.

Data bank

This activity of the TDC is based on the created thermodynamics data bank.
For over 25 years primary experimental thermodynamic data are collected on the basis of the open world literature and evaluated at the following levels: primary experimental data, selected data, recommended data, and parameters of the selected equations.
Selected and recommended data are prepared after critical evaluation. Parameters of equations are calculated for selected and recommended data for a given range of temperature. For process simulators binary interaction parameters for mixtures are offered in a format suitable for direct use.

The Data Bank contains experimental data of thermophysical properties both for pure organic substances and for binary and ternary mixtures.

1. Pure substance properties: triple point temperature, triple point pressure, cryoscopic constant, critical temperature, critical pressure, critical volume, critical density, critical compressibility factor, phase transition enthalpy, standard state enthalpy for formation, density, equilibrium pressure, heat capacity at saturation, heat capacity at constant pressure, heat capacity at constant volume, enthalpy of vaporizatiom at saturation, enthalpy of transition from Ph1 to Ph2, enthalpy, entropy, Gibbs energy, surface tension, viscosity, kinematic viscosity, velocity of sound, thermal conductivity, thermal diffusivity, second virial coefficient, third virial coefficient, refractive index, coefficient of expansion, isothermal compressibility, adiabatic compressibility, thermal pressure coefficient.
2. Mixture properties: vapor-liquid equilibria, liquid-liquid equilibria, solid-liquid equilibria, solubilities of gases in liquids, heat of mixing, excess volume, and excess heat capacity.

The traditional Floppy Book software is applied as a managing program for the all data bases in the TDC. The user friendly Floppy Book program, working under Windows on IBM PC compatible computers, allows to select the following options:

- selection of system and property by a visual or a pattern match search
- selection of data sets
- display of the experimental results in tabular form
- graphical presentation
- calculation when equation parameters are available
- regression and prediction of the data
- saving of experimental and calculated results to external files.

The TDC offers packets containing requested data together with the floppy book software.

Contact persons:

Dr. Adam Skrzecz
phone: +(48 22) 343-3306; email: skrzecz@ichf.edu.pl

VII. Department of Electrode Processes

Head: Associate Professor Marcin Opałło

The Department's research topics concentrate on the processes at the electrode/electrolyte interface. Both experimental and theoretical work is conducted. Lately attempts have been made to obtain or modify new electrode materials and electrolytes.

One of the Department's most important achievements in the last years has been proposing clathrate hydrates of tetraalkylammonium hydroxides as a new group of solid electrolytes with high conductivity in low temperatures (100–200 K). Cryoelectrochemical research in these electrolytes allowed to understand better the reaction of hydrogen evolution and properties of thin film nickel hydroxide electrode. Another important issue was the proposal of polysilicate matrix obtained through the sol-gel method and modified with organic liquids as new electrolytes and electrodes. Electrodes modified with hydrophobic redox liquids seem to be especially interesting as they show high current density and sensitivity to electro-inactive ions. Investigations were also conducted on the gold electrode as a model system of stable electrode/electrolyte interface and its electrocatalytic properties in systems applied in fuel cells. The influence of the surface structure of the electrode on the process of electrocatalytic methanol oxidation was determined. Transport of hydrogen in metal served as an example to describe guest transport in the elastic matrix of a host, with particular attention paid to nonlinearity of this process. Methodology of impendance spectroscopy and, more widely, transfer function spectroscopy was also developed. Theoretical research was done including an application of the field theory to work out an electrolyte model describing behaviour of ions at charged walls.

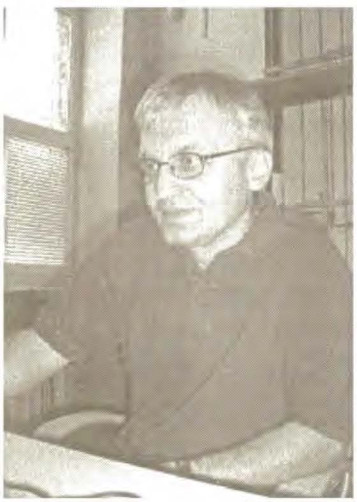
At present most employees at the Department are engaged in a research project connected with electrodes based on polysilicate matrixes and other meso- and nanoporous materials. These systems modified with redox, hydrophobic or ionic liquids may be applied in such electrochemical systems as sensors of ions or gaseous phase substances. We are also interested in transport phenomena and the mechanism of electrode reactions in these matrixes.

We also develop a model description of coulombic systems based on statistical field approach to explain the behaviour of inhomogeneous electrolyte systems at a hard wall as well as of bulk electrolyte. We use numerical simulations of cellular automata type to model surface development in corrosion and growth processes. It may help in designing surface treatment procedures to obtain surface with the requested roughness and other structural properties. We are going to continue our work on the description of guest transport in the host network elastic matrix.

We are beginning biomimetic research. It will concern binding toxic proteins such as, *e.g.* cholera toxin, through lipid bilayers and distribution of polymers found in nature, *e.g.* lignins. The results of this research will not only help to understand processes occurring in nature but they may also be important in biotechnology. Moreover, we have taken up investigation of electrode reactions catalysed by enzymes. They are to result in the creation of a model of a miniature biocompatible fuel biocell producing electric energy from glucose and oxygen – substances present in live organisms.

Some of the research projects mentioned above are realised in cooperation with research teams from other departments of the Institute of Physical Chemistry of PAS, institutes of PAS and universities in Poland and scientific centres in Bulgaria, France, Greece, Canada, United States and Great Britain.

Marcin Opałło, Associate Professor



M. Sc., 1980 – Department of Chemistry, Warsaw University
Ph.D., 1987 – Institute of Physical Chemistry, Warsaw
D.Sc., 1999 – Institute of Physical Chemistry, Warsaw

Education and training:

1987–1989 – Pharmaceutical Institute, Tohoku University, Sendai, Japan
1990–1992 – University of California, Davis, USA
1994 – Forschungzentrum Julich, Julich, Germany

Professional affiliations:

- Polish Chemical Society (since 1979)
- International Society for Electrochemistry (since 2000)

Research areas:

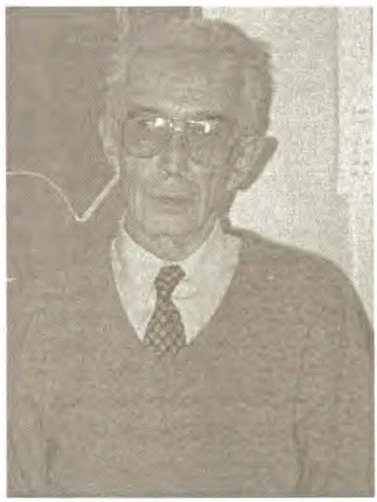
- Electrode reactions
- Sol-gel chemistry
- Solid electrolytes
- Redox and ionic liquids

Selected papers

1. Opałło M. and Kapturkiewicz A., "Solvent effect on the kinetics of the electrooxidation of phenothiazine", *Electrochim. Acta*, **30**, 1301–1306 (1985).
2. Opałło M., "The solvent effect on the electrooxidation of 1,4-phenylenediamine", *J. Chem. Soc. Far. Trans. I*, **82**, 339–346 (1986).
3. Fawcett W.R., Opałło M., Fedurco M. and Lee J.W., "The kinetics and thermodynamics of the electroreduction of buckminsterfullerene in benzonitrile", *J. Am. Chem. Soc.*, **115**, 196–199 (1993).
4. Fawcett W.R. and Opałło M., "The kinetics of heterogeneous electron transfer reactions in polar solvents", *Angewandte Chem. Int. Ed.*, **33**, 2131–2144 (1994).
5. Opałło M. and Prokopowicz A., "Electrochemical hydrogen evolution in hydroxide hydrate down to 110 K", *Electrochem. Commun.*, **2**, 23–28 (2000).
6. Opałło M. and Kukulka J., "The electrochemical redox reaction in silica sol-gel glass, with embedded organic electrolyte", *Electrochem. Commun.*, **2**, 394–399 (2000).
7. Opałło M. and Saczek-Maj M., "Electroactive ceramic carbon electrode impregnated with organic liquid", *Electrochemistry Commun.*, **3**, 306-311 (2001).
8. Opałło M. and Sączek-Maj M., "Carbon ceramic electrode modified with redox liquid", *Chem. Commun.*, 448–449 (2002).
9. "Solid electrolyte based on silicate matrix functionalised with tetraalkylammonium group solvated by organic solvent", Opałło M., Niedziółka J., Sączek-Maj M., Shul G., Utzig E., Mrowiec-Białoń J., Stygar J. and Wieczorek W., *Electrochimica Acta*, **48**, 4149–4155 (2003).
10. Stabilising electrode/redox liquid/aqueous solution system with hydrophobic silicate film", Niedziółka J. and Opałło M., *Electrochem. Commun.*, **6**, 475–479 (2004).

Total number of publications: 68

Piotr Żółtowski, Associate Professor



M.Sc., 1959 – Department of Chemistry, Technical University of Warsaw
Ph.D., 1967 – Institute of Physical Chemistry, Warsaw
D.Sc., 1989 – Institute of Physical Chemistry, Warsaw

Education and training:

1971 – University of Belgrade, Yugoslavia

Professional affiliations:

- Polish Chemical Society
- International Society of Electrochemistry
- Electrochemical Society

Research areas:

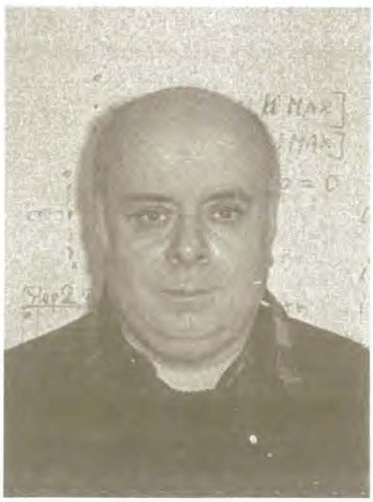
- Mechanisms and kinetics of reactions of at solid electrodes
- Metal-hydrogen systems
- Transport of guest in solid host
- Impedance spectroscopy

Selected papers

1. Żółtowski P., "The error function for fitting of models to immitance data", *J. Electroanal. Chem.*, **178**, 11–19 (1984).
2. Żółtowski P., "An immitance study of the mechanism of hydrogen reactions on the tungsten carbide electrode, I & II", *J. Electroanal. Chem.*, **260**, 269–301 (1989).
3. Żółtowski P., "A new approach to the measurement modelling in electrochemical impedance spectroscopy", *J. Electroanal. Chem.*, **375**, 45–57 (1994).
4. Żółtowski P., "The power of reparametrization of measurement models in electrochemical impedance spectroscopy", *J. Electroanal. Chem.*, **424**, 173–178 (1997).
5. Borkowska Z., Opałło M., Tymosiak-Zielińska A. and Żółtowski P., "Tetraalkylammonium clatrate hydrates in interfacial electrochemistry", *Colloids and Surfaces A*, **134**, 67–73 (1998).
6. Żółtowski P., "On the electrical capacitance of interfaces revealing constant phase element behaviour", *J. Electroanal. Chem.*, **443**, 149–154 (1998).
7. Żółtowski P., "Effects of self-induced mechanical stress in hydrogen sorption by metals, by EIS", *Electrochim. Acta*, **44**, 4415–4429 (1999).
8. Żółtowski P., "Diffusion of hydrogen in self-stressed metals – Transfer function spectroscopy approach", *J. Electroanal. Chem.*, **501**, 89–99 (2001).
9. Żółtowski P. and Makowska E., "Diffusion coefficient of hydrogen in α-phase palladium and palladium-platinum alloy", *Phys. Chem. Chem. Phys.*, **3**, 2935–2942 (2001).
10. Żółtowski P., "Concentration transfer function of hydrogen diffusion in self-stressed metals", *J. Electroanal. Chem.*, **512**, 64–73 (2001).
11. Legawiec B. and Żółtowski P., "Effects of Self Stress on the Transport of Guest Species in Solids: Transport of Hydrogen in Metals", *J. Phys. Chem. B*, **106**, 4933–4940 (2002).
12. Żółtowski P., "Sensitivity of Transfer Functions of Transport of Hydrogen in Elastic Metals to the Uncertainty of Their Parameters", *Acta Mater.*, **51**, 5489–5497 (2003).

Total number of publications: 43

Janusz Stafiej, Research Associate



M.Sc., 1980 – Department of Physics, University of Warsaw
Ph.D., 1991 – Institute of Physical Chemistry, Warsaw
D.Sc., 2002 – Institute of Physical Chemistry, Warsaw

Education and training:

1993 – Structure et Réactivité aux Interfaces, Université P. et M. Curie Paris VI, France (Fellowship of the European Community)

2002 – Laboratoire Analyse et Environnement, Université d'Evry, Evry Val d'Esonne, France (Research position of the CNRS)

Research areas:

- Field theoretical approach to coulombic systems.
- Cellular automata based approach to modeling of corrosion processes

Selected papers

1. Di Caprio D., Stafiej J. and Badiali J.P., "Density field theory for a fluid interacting with the Yukawa potential. Role of the ideal entropy", *Mol, Phys.*, **101**, 3197–3202 (2003).
2. di Caprio D., Borkowska Z. and Stafiej J., "Specific ionic interactions within a simple extension of the Gouy-Chapman theory including hard sphere effects", *J. Electroanal Chem.*, **572**, 15 (2004).
3. di Caprio D., Stafiej J. and Borkowska Z., "Anomalous temperature dependence of differential capacity at un uncharged interface with Debye-Hűckel electrolyte", *J. Electroanal Chem.*, accepted.
4. Taleb A., Chausse A., Dymitrowska M., Stafiej J. and Badiali J.P., "Simulations of corrosion and passivation phenomena: Diffusion feedback on the corrosion rate", *J. Phys. Chem. B*, **108**, 952–958 (2004).
5. Saunier J., Chausse A., Stafiej J. and Badiali J.P., "Simulations of diffusion limited corrosion at the metal| environment interface", *J. Electroanal Chem.*, **563**, 239–247 (2004).
6. Saunier J., Chausse A., Dymitrowska M., Stafiej J. and Badiali J.P., "Diffusion, interactions and universal behavior in a corrosion growth model", *J. Electroanal Chem.*, accepted.

Total number of publications: 31

VIII. Department of Electrochemical Oxidation of Gaseous Fuels

Head: Professor Leszek Suski

At present, Department of Electrochemical Oxidation of Gaseous Fuels is the only unit of the Institute located outside of Warsaw. The Department has been established in 1990, bearing the name of Department of Molten Salts. Before 1990 the unit had a status of laboratory. The Department staff conducted physicochemical research of metal – its molten halide systems (*e.g.* Cd-CdX_2, K-KX, (X=Cl, Br, J) such as excess mole volume, surface tension, electric conductivity and viscosity. For this purpose a number of measurement techniques were devised such as, radiometric method of determining changes of molar volume in a two-component compound (developed in cooperation with Institute of Nuclear Technology of University of Science and Technology in Cracow). These techniques have acquired wide recognition and thanks to that the team was invited to participate in the Program of Standards for Molten Salts led by Molten Salt Data Center in Resenclear Polytechnic Institute, Troy, N.Y., USA and by the National Bureau of Standards in Washington.

Chemical and electrochemical basis of high-temperature carbonate fuel cells have become the main research topic in last years. In the last decade, the research in this scope was financed not only by the State Committee for Scientific Research but also by US – Poland Cooperation Fund II (cooperation with Gas Technology Institute, Des Plaines, Illinois) and Japanese programme NEDO (cooperation with Tohoku University, Sendai). A number of publications in the scope of chemistry and electrochemistry of molten carbonates dealt with the results of research on modelling of processes occurring in porous electrodes of fuel cell, kinetics of electrode hydrogen oxidation processes, reduction of oxygen electrode materials and acid-base equilibrium. The team of Department VIII is the only research group in Poland which has sophisticated basis and experience for laboratory realisation of fuel cells.

At present, the research conducted in the Department is directed toward processes of electrochemical oxidation of fuels at an interface electrode/high temperature solid electrolyte, for example ZrO_2 stabilised by yttrium oxides. These works have a character of electrochemical fundamental research but they were initiated by the vital problems of the high temperature fuel cells with solid oxide electrode. In connection with an idea of one-chamber fuel cell, the investigations in the scope of thermodynamics and kinetics of methane oxidation in electrode with catalytic properties/solid oxide electrolyte systems were carried out. The special emphasis was put on system of two different electrodes in atmosphere of gaseous mixtures fuel + oxygen (*e.g.* $CH_4 + O_2$). Particularly promising results have been obtained with the use of electrode materials based on perovskites and ceramic materials of mixed ion-electron conductivity based on CeO_2. An oxygen electrode in a solid polymer electrolyte will be investigated through electrochemical impedance spectroscopic method with the use of ultramicroelectrodes.

Separate research path is connected with works on simulative solving of problems in kinetics and mechanism of complex electrode processes. Alternative ways of adaptation aimed at further improvement of solutions will be investigated in the scope of a development of algorithms of computational electrochemistry.

Leszek Suski, Professor

M.Sc., 1952 – Department of Sciences – Jagiellonian University of Cracow.

Ph.D., 1957 – Department of Metallurgy, technical University of Mining and Metallurgy, Cracow.

D.Sc., 1968 – Institute of Physical Chemistry, Warsaw.

Professor of Chemistry 1974 – Institute of Physical Chemistrys, Warsaw.

Emeritus Professor of Chemistry 2001 – Institute of Physical Chemistry, Warsaw.

Professional experience:

- 1959/60 Istituto di Fisica Chimica ed Elettrochimica del Politechnico di Milano (Profesor Roberto Piontelli).
- 1970 Institute of Physical Chemistry of the Polish Academy of Sciences, Head of Department of Physical chemistry of Molten Salts (in Cracow)
- 1981 Université de Marseille , visiting professor.
- 2000 Institute of Physical Chemistry of the Polish Academy of Sciences, Head of Department of Electrochemical Oxidation of gaseous Fuels.

Professional affiliations:

- Polish Chemical Society (since 1958).
- The Electrochemical Society, Inc., (USA, since 1993).

Research areas:

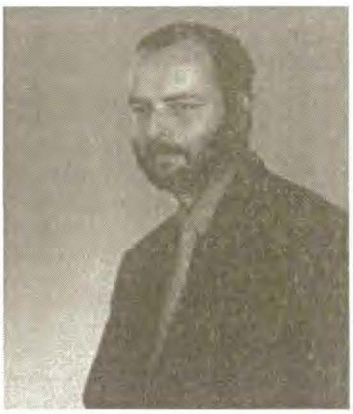
Chemistry and electrochemistry of molten salts, chemistry of metal – its molten salt systems, chemistry of molten carbonates as relevant to Molten Carbonate Fuel cells, electrode processes of fuels (hydrocarbons) oxidation at solid oxide ionic conductors.

Selected papers

1. Suski L. and Mościński J., "A correlation of the excess molar volumes of solution of cadmium and bismuth in their molten halides", *J. Phys. Chem.*, **75**, 3620 (1971).
2. Jewulski J. and Suski L., "Chemical Equilibrium diagrams relevant to the molten carbonate Fuell Cell – CHO gas + molten alkali carbonates + metal oxides heterogeneous systems", Thermochemical Data for Technology, Series B, Polish Academy of Sciences – Institute of Physical Chemistry, Warsaw, 1985.
3. Jewulski J. and Suski L., "Model of isotropic anode in the molten carbonate fuel cell", *J. Appl. Electrochem.*, **14**, 135 (1984).
4. Suski L., Godula-Jopek A. and Obłąkowski J., "Wetting of Ni and NiO by alternative molten carbonate fuel cell electrolytes, I. Influence of gas atmosphere", *J. Electrochem. Soc.*, **146**, 4048 (1999).
5. Godula-Jopek A. and Suski L., "Wetting of Ni and NiO by alternative molten carbonate fuel cell electrolytes, I.I. Influence of the electrode overpotential", *J. Electrochem. Soc.*, **147**, 910 (2000).
6. Suski L. and Ruggiero M., "Electrochemical determination of the thermodissociation equilibrium in molten Li+Na carbonates", *Electrochem. Solid-State Letters*, **2**, 579 (1999).
7. Suski L. and Tarniowy M., "The phase stability of solid $LiAlO_2$ used for the electrolyte matrix of molten carbonate fuel cell", *J. Mater. Sci.*, **36**, 5119 (2001).
8. Danek V., Tarniowy M. and Suski L., "Kinetics of the $\alpha\gamma$-phase transformation in $LiAlO_2$ under various atmospheres, within the 1073–1173 K temperature range", *J. Mater. Sci. Chem.*, **39**, 2429 (2004).
9. Suski L., Kołacz J., Mordarski G. and Ruggiero M., "Determination of open-circuit-potentials at gas/electrode/YSZ boundary *vs.* molten carbonate reference electrode at medium temperatures. I. Potentials of Au and Pt electrodes in O_2 and H_2+H_2O atmospheres", *Electrochim Acta*, in print.
10. Mordarski G., Suski L., Ruggiero M., Kołacz J. and Wyrwa J., "Determination of open-circuit-potentials at gas/electrode/YSZ boundary *vs.* molten carbonate reference electrode at medium temperatures. II. Potential response of Au, Pt and Ni-cermet electrodes in H_2+O_2 and CH_4+O_2 gas mixtures", *Electrochim Acta*, in print.

Total number of publications: *ca* 100

Lesław Bieniasz, Research Associate



M.Sc., 1980 – Department of Electrotechnics, Automatics and Electronics, University of Mining and Metallurgy, Cracow

Ph.D., 1987 – Institute of Physical Chemistry of the Polish Academy of Sciences, Warsaw.

D.Sc., 2001 – Department of Chemistry, University of Aarhus, Aarhus, Denmark

Education and training:

- 1984 – Institute of Electrochemistry of the USSR Academy of Sciences, Moscow, USSR
- 1992/1993 – Department of Chemistry, University of Aarhus, Aarhus Denmark
- 1996 – Department of Chemistry, University of Aarhus, Aarhus Denmark
- 1997 – Institute of Organic Chemistry, Tübingen University, Tübingen, Germany
- 1998 – Institute of Organic Chemistry, Tübingen University, Tübingen, Germany
- 1999 – Centre Commissariat a l'Energie Atomique (C.E.A.), Saclay, France
- 2000 – Department of Chemistry, University of Aarhus, Aarhus Denmark
- 2002 – Department of Chemistry, Saitama University, Saitama, Japan

Research areas:

Computational electrochemistry; development of computational approaches to solving problems of electrochemical kinetics, including digital simulation of transient electrochemical experiments and computer-aided electrochemical data analysis. Theory of transient methods. Formal kinetics of complex electrochemical reactions and phenomena, including electrocatalytic reactions.

Selected papers

1. Bieniasz L.K., Britz D., "Recent Developments in Digital Simulation of Electroanalytical Experiments" (Review), *Pol. J. Chem.*, **78**, 1195–1219 (2004).
2. Bieniasz L.K. "Towards Computational Electrochemistry - A Kineticist's Perspective", in Modern Aspects of Electrochemistry, B.E. Conway, R. E. White (Eds.), vol. 35, Kluwer Academic/Plenum Publishers, New York, 2002, pp. 135–195.
3. Karantonis A., Bieniasz L. and Nakabayashi S. "The Combined Unidirectional and Local Coupling in a Spatially One-Dimensional Model of Oscillatory Metal Electrodissolution. Patch-Adaptive Simulation Study", *Phys. Chem. Chem. Phys.*, **5**, 1831-1841 (2003).
4. Bieniasz L.K. "Analytical Formulae for Chronoamperometry of a Charge Neutralisation Process under Conditions of Linear Migration and Diffusion", *Electrochem. Commun.*, **4**, 917–921 (2002).
5. Bieniasz L.K. "Extension of the Thomas Algorithm to a Class of Algebraic Linear Equation Systems Involving Quasi-Block-Tridiagonal Matrices with Isolated Block-Pentadiagonal Rows, assuming Variable Block Dimensions", *Computing*, **67**, 269–285 (2001)., *Computing*, **70**, 275–275 (2003) (erratum).
6. Bieniasz L.K., Bureau C. "Use of Dynamically Adaptive Grid Techniques for the Solution of Electrochemical Kinetic Equations. Part 7. Testing of the Finite-Difference Patch-Adaptive Strategy on Example Models with Moving Reaction Fronts, in One-Dimensional Space Geometry", *J. Electroanal. Chem.*, **481**, 152–167 (2000)., *J. Electroanal. Chem.*, **565**, 135–135 (2004) (corrigendum).
7. Bieniasz L.K., Speiser B. "Use of Sensitivity Analysis Methods in the Modelling of Electrochemical Transients Part 3. Statistical Error/Uncertainty Propagation in Simulation and in Nonlinear Least-Squares Parameter Estimation", *J. Electroanal. Chem.*, **458**, 209–229 (1998).
8. Bieniasz L.K. "ELSIM - A Problem Solving Environment for Electrochemical Kinetic Simulations. Version 3.0 - Solution of Governing Equations Associated with Interfacial Species, Independent of Spatial Coordinates or in One-dimensional Space Geometry", *Comput. Chem.*, **21**, 1–12 (1997).
9. Tomczyk P. and Bieniasz L.K., "Kinetics of the Oxygen Electrode Reaction in Molten (Li / Na) Carbonate Eutectic. Part III: Quantitative Analysis of the Linear Scan Voltammetric Curves for the First Reduction Process at Au Electrodes", *J. Electroanal. Chem.*, **304**, 111–121 (1991).
10. Bieniasz L.K. "The Linked Mechanism of the Hydrogen Electrode Reaction in Molten Carbonates", *J. Electroanal. Chem.*, **197**, 387–393 (1986).

Total number of publications: 62

Piotr Tomczyk, Research Associate

M.Sc., 1970 – Jagiellonian University, Cracow
Ph.D., 1977 – Institute of Physical Chemistry, Warsaw
D.I.C., 1980 – Imperial College of Science and Technology, London
D.Sc., 1997 – Institute of Physical Chemistry, Warsaw

Education and training:

1973 – Centre of Physical Chemistry, Bucharest, Romania
1979/80 – Imperial College of Science and Technology, London, Great Britain
1988 – Central Electrochemical Institute, Karaikudi, India
1990 – Institute of General and Inorganic Chemistry UAS, Kiev, Ukraine
1993/4 – Tohoku University, Sendai, Japan
1998/9 – Tohoku University, Sendai, Japan

Professional affiliations:

- AGH University of Science and Technology, Cracow

Research areas:

- Electrochemistry and chemistry of molten salts
- Fuel cells

Selected papers

1. Suski L. and Tomczyk P., "Application of hard-sphere theory to the compressibilities of some fused-salt binary mixtures", *J. Chem. Thermodynamics*, **13**, 803 (1981).
2. Tomczyk P. and Mordarski G., "Kinetics of the oxygen electrode reaction in molten Li + Na carbonate eutectic. Part 1. Linear voltammetric and chronoamperometric data for the reduction process at Au electrodes", *J. Electroanal. Chem.*, **304**, 85 (1991).
3. Tomczyk P., "Kinetics of the oxygen electrode reaction in molten Li + Na carbonate eutectic. Part 7. Effect of CO_2 partial pressure on the linear scan voltammetric response for the reduction process at Au electrodes", *J. Electroanal. Chem.*, **379**, 353 (1994).
4. Tomczyk P., Wyrwa J. and Mosiałek M., "Electrochemical behaviour of $Li_xNi_{1-x}O$ in molten Li_2CO_3 + Na_2CO_3 eutectic", *J. Electroanal. Chem.*, **463**, 78 (1999).
5. Tomczyk P., Ono Y., Hisamitsu Y., Mohamedi M. and Uchida I., "Fractal Approach to Surfaces Formed during In Situ Oxidation of Some Metals in Molten Carbonates", *Electrochem. and Solid State Letters*, **2**, 431 (1999).
6. Tomczyk P. and Mosiałek M., "Investigation of the oxygen electrode reaction in basic molten carbonates using electrochemical impedance spectroscopy", *Electrochim. Acta*, **46**, 3023 (2001).

Total number of publications: 32

IX. Department of Photochemistry and Spectroscopy

Head: Professor Jacek Waluk

Two research topics dominate in the Department – investigations of the structure and reactivity of molecules in electronically excited states and application and development of new spectroscopic techniques with high spectral, spatial or temporal resolution.

The most important achievements of the Department in recent years (some result from research started in 1970s) include, among others:

- the discovery and comprehensive investigation of a new class of molecular excited states (TICT states) in systems of the electron donor-acceptor type (D-A) formally connected by a single bond;
- the demonstration that Marcus theory may be applied for uniform quantitative characterisation of intramolecular radiative and nonradiative electron transfer;
- the investigation of the electronic structure and geometry of large π -electron D-A systems;
- the investigation of phenomena (including intramolecular and intermolecular proton transfer) induced by hydrogen bonds in bifunctional aromatic molecules;
- the elucidation of processes of phototautomerism and photochromism for certain Schiff bases;
- the elucidation of factors governing electrochemiluminescense (ECL) and the quest for systems characterised by particularly high ECL efficiency;
- the study of the chemistry and spectroscopy of unstable carbon-nitrogen chain molecules of astrophysical significance;
- the development of polarized spectroscopic methodology allowing:
  * the analysis of linear dichroism spectra for low-symmetry molecules;
  * the determination of chemical reaction rate based on the analysis of luminescence anisotropy and linear dichroism spectra;
  * the interpretation of electronic absorption and magnetic circular dichroism spectra of aromatic molecules (particularly for isomeric and expanded porphyrins);
- the development of IR, UV-VIS spectroscopy and mass spectrometry methods which allow:
  * the investigation of pico- and femtosecond kinetics of photoinduced processes of charge transfer and phototautomerisation;
  * the investigation of systems isolated in the gas phase in supersonic molecular beams or in low-temperature matrices of noble gases;
  * the luminescence of single molecules;
- the elaboration of a computational method that allows one to predict the structure of microenvironments of organic and inorganic chromophores in noble gas matrices and their electronic and infrared spectra.

In near future, we are going to take up a range of new tasks connected both with fundamental and applied research. Among others, the following investigations are planned in connection with:

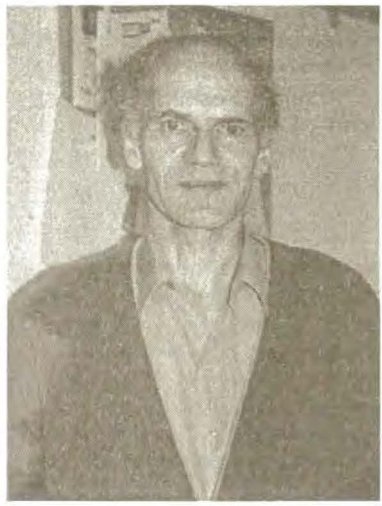
- synthesis, spectroscopy and phototherapeutic properties of porphyrins;
- phototautomerisation in single molecules;
- laboratory astrochemistry;
- photoinduced charge transfer and phototautomerisation in model systems isolated in supersonic molecular beams;
- application of femtosecond time-resolved methods to the investigation of electron and proton transfer mechanisms;
- practical use of charge separation processes (with placement of chromophores in solid phases);
- synthesis and properties of sensors;
- photochemistry on surfaces.

We are going to further improve our research capacity through the development of femtosecond emission spectroscopy, coupling of laser flash photolysis and NMR detection, application of spectroscopy with the use of polarised light for research on the kinetics of phototautomerisation or relaxation processes in cryogenic matrices, elaboration of new methodology for matrix preparation (multi-laminar deposition) and development of single molecule spectroscopy.

The Department has rich international cooperations with the participation of scientists from Germany, Denmark, Austria, Holland, France, United Kingdom, Switzerland, Spain, USA, Brazil, Japan, Taiwan, Bulgaria, Ukraine, Belarus and Russia.

The Department is a coordinator of the Centre of Excellence CPM (Centre for Photoactive Materials) in the framework of the 5th Framework Programme of the European Union, and it is the main performer of the Centre tasks.

Jacek Waluk, Professor



M. Sc., 1974 – Department of Chemistry, University of Warsaw
Ph.D., 1979 – Institute of Physical Chemistry, Warsaw
D Sc., 1987 – Institute of Physical Chemistry, Warsaw
1998, Professor – Institute of Physical Chemistry, Warsaw

Professional experience:

1980 – University of Utah, USA
1984, 1985, 1986 – Royal Danish School of Educational Studies, Denmark
1987, 1991, 1992, 1993 – Technical University of Berlin, Germany
1993, 1994, 1995 – University of Roskilde, Denmark
1999, 2001 – Colorado School of Mines/National Renewable Energy Laboratory, USA
2000 – University of Colorado, USA

Professional affiliations:

- European Photochemistry Association (Chairman, 2000–2004)
- Polish Chemical Society
- American Chemical Society
- Society for Advancement of Science and Arts (TPKN)
- International Society of Porphyrins and Phthalocyanines
- Advisory/ownership boards: *J. Luminescence, Photochemical and Photobiological Sciences, Chemical Physics*

Research areas:

- Physical Organic Chemistry (proton and electron transfer, structure and reactivity of azaaromatics and porphyrin isomers, hydrogen bonding, conformational equilibria)
- Spectroscopy and Photophysics (electronic absorption/emission, IR/Raman, matrix isolation, linear and magnetic circular dichroism, time-resolved techniques)
- Theoretical Chemistry

Selected papers

1. Piwoński H., Stupperich C., Hartschuh A., Sepioł J., Meixner A. and Waluk J., "Imaging of tautomerism in a single molecule", *J. Am. Chem. Soc.*, (2005).
2. Gorski A., Köhler T., Seidel D., Lee J.T., Orzanowska G., Sessler J.L. and Waluk J., "Electronic structure, spectra and magnetic circular dichroism of cyclohexa-, cyclohepta-, and cyclooctapyrrole", *Chem. Eur. J.*, (2005).
3. Kijak M., Zielińska A., Chamchoumis C., Herbich J., Thummel R.P. and Waluk J., "Conformational equilibria and photoinduced tautomerization in 2-(2′-pyridyl)pyrrole", *Chem. Phys. Lett.*, **400**, 279–285 (2004).
4. Waluk J., "Hydrogen-bonding-induced phenomena in bifunctional heteroazaaromatics", *Acc. Chem. Res.*, **36**, 832–838 (2003).
5. Kyrychenko A. and Waluk J., " Molecular dynamics simulations of matrix deposition I: Site structure analysis for porphyrin in argon and xenon", *J. Chem.Phys.*, **119**, 7318–7327 (2003).
6. Dobkowski J., Wójcik J., Koźmiński W., Kołos R., Waluk J. and Michl J., "Syn-anti photoisomerization in 2-(N-methyl-N-isopropylamino)-5-cyanopyridine", *J. Am. Chem. Soc.*, **124**, 2406–2407 (2002).
7. Waluk J., "Conformational aspects of intra- and intermolecular excited state proton transfer"; *Conformational Analysis of Molecules in Excited States* (J. Waluk, Ed.); Wiley-VCH, 57–111 (2000).
8. Kyrychenko A., Herbich J., Wu F., Thummel R.P. and Waluk J., " Solvent-induced syn-anti rotamerization of 2-(2′-pyridyl)indole and the structure of its alcohol complexes ", *J. Am. Chem. Soc.*, **122**, 2818–2827 (2000).
9. Kyrychenko A., Stepanenko Y. and Waluk J., " Molecular dynamics and DFT studies of intermolecular hydrogen bonds between bifunctional heteroazaaromatic molecules and hydroxylic solvents", *J. Phys. Chem. A*, **104**, 9542–9555 (2000).
10. Kyrychenko A., Herbich J., Izydorzak M., Wu F., Thummel R.P. and Waluk J., " Role of ground state structure in photoinduced tautomerization in bifunctional proton donor-acceptor molecules: 1H-pyrrolo[3,2-*h*]quinoline and related compounds", *J. Am. Chem. Soc.*, **121**, 11179–11188 (1999).

Total number of publications: 140

Anna Grabowska, Professor Emeritus

M.Sc., 1954 – Faculty of Chemistry, Warsaw University
Ph.D., 1961 – Faculty of Chemistry, Warsaw University
D.Sc., 1969 – Institute of Physical Chemistry, Warsaw
Professor, 1988 – Institute of Physical Chemistry, Warsaw

Research abroad:

1964 – Free University, Amsterdam, The Netherlands
1971–1972 Cambridge University, United Kingdom
1987–1988 Institute for Molecular Science, Okazaki, Japan
1988 – Université de Bordeaux I, Talence, France

Professional affiliations:

- Polish Chemical Society
- Society for Advancement of Science and Arts (TPKN)
- European Photochemistry Association

Research areas:

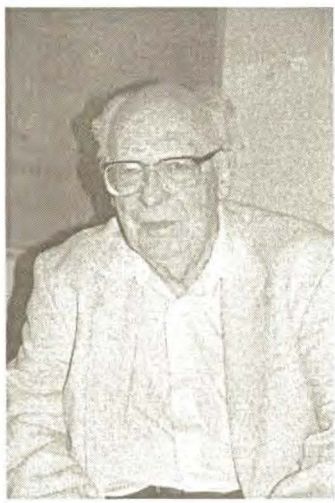
- Physical chemistry
- Molecular spectroscopy
- Photochemistry
- Photophysics

Selected papers

1. Grabowska A., Mordziński A., Tamai N. and Yoshihara K., "Reversible intramolecular proton-transfer reactions of electronically excited "double" benzoxazoles: a direct observation of the effect of intrinsic barrier", *Chem. Physics Letters*, **169**, 450–456 (1990).
2. Grabowska A., Mordziński A., Kownacki K., Gilabert E. and Rullière C., "Picosecond transient absorption and gain spectra of the excited internally H-bonded benzoxazole derivatives. Experimental proof of the thermal activation of the intramolecular proton transfer", *Chem. Physics Letters*, **177**, 17–22 (1991).
3. Borowicz P., Grabowska A., Wortmann R. and Liptay W., "Tautomerization in fluorescent states of bipyridyl-dioles. A direct confirmation of the intramolecular double proton transfer by electrooptical emission measurements", *J. Luminescence*, **52**, 265–273 (1992).
4. Grabowska A. and Kaczmarek Ł., "Bipyridyl-diols, molecules undergoing an internal double proton transfer reaction in electronically excited states", *Polish J. Chem.*, **66**, 715–731 (1992).
5. Grabowska A., "Proton transfer reaction prepared by the hydrogen bonds in electronically excited polyatomic molecules", Proc. Internat. Research Workshop "Ultrafast Reaction Dynamics and Solvent Effects"; Abbaye de Royaumont, 1993, (Y. Gauduel, P.J. Rossky, eds.), American Institute of Physics, New York, 1994; pp. 255–271.
6. Kownacki K., Mordziński A., Wilbrandt R. and Grabowska A., "Laser-induced absorption and fluorescence studies of photochromic Schiff bases", *Chem. Physics Letters*, **227**, 270–276 (1994).
7. Marks D., Zhang H., Borowicz P., Grabowska A. and Glasbeek M., "Femtosecond intramolecular proton transfer in photoexcited mono- and dienol derivatives of bipyridine", *Chem. Physics Letters*, **309**, 19–28 (1999).
8. Wortmann R., Lebus S., Reis H., Grabowska A., Kownacki K. and Jarosz S., "Spectral and electrooptical absorption and emission studies on internally hydrogen-bonded benzoxazole "double" derivatives: 2,5-bis(benzoxazolyl)hydroquinone (BBHQ) and 3,6-bis(benzoxazolyl)-pyrocatechol (BBPC). Single versus double proton transfer in the excited BBPC revisited", *Chem. Physics*, **243**, 295–304 (1999).
9. Zgierski M.Z. and Grabowska A., "Photochromism of salicylideneaniline (SA). How the photochromic transient is created ? A theoretical approach", *J. Chem. Physics*, **112**, 6329–6337 (2000).
10. Ziółek M., Kubicki J., Maciejewski A., Naskręcki R. and Grabowska A., "An ultrafast excited state intramolecular proton transfer (ESPIT) and photochronism of salicylideneaniline (SA) and its "double" analogue salicylaldehyde azine (SAA). A controversial case", *Phys. Chem. Chem. Phys.*, **6**, 4682–4689 (2004).

Total number of publications: about 70

Zbigniew R. Grabowski, Professor Emeritus



Professional affiliation: Polish Academy of Sciences

M.Sc., 1950 – Chemistry, Warsaw University

Ph.D., („Cand.Sci."), 1955 – Chemistry, Warsaw University

Reader (Docent), 1957, Faculty of Science, Warsaw University

Professor, 1965 – Institute of Physical Chemistry, Warsaw

Dr h.c., 1993 – Université de Fribourg, Switzerland

Professor, College of Science, Warsaw, 1993–2001

Research abroad:

1956 – Exchange scientist, Inst. of Physical Chemistry, AS USSR, Moscow

1959 – Rockefeller Fellow, Techn. Univ., Stuttgart, Germany

1971–1972 Overseas Fellow, Churchill College, Cambridge, U.K

1986 – Visiting Professor, Universités Romandes en Suisse

1986 – Professeur Associé, Université de Paris-Sud, Orsay, France

1987 – Professeur Associé, Université de Bordeaux I, Talence, France

1987–1988 – Visiting Professor, Institute for Molecular Science, Okazaki, Japan

1989 – Visiting Professor, Katholieke Universiteit Leuven, Belgium

Professional affiliations:

- Polish Chemical Society (since 1948; honorary member since 1987)
- Farady Society (1959–82)
- German Academy of Sciences "Leopoldina" (since 1977)
- Society for the Advancement of Science and Arts (TPKN) (since 1980; 1980–92 chairman of the Council; 1992–94 president)
- Warsaw Learned Society (since 1982)
- European Photochemistry Association

Research areas:

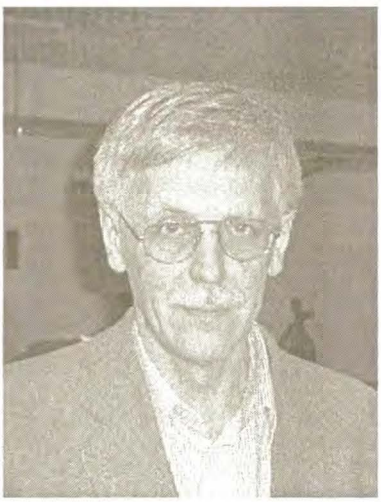
- Electrochemistry: kinetics, electric field effects; stereochemistry (1949–70)
- Chemistry of free radicals: kinetics and equilibria, spectra (1960–77)
- Instrumental methods: time-resolved spectroscopy (1959–95)
- Electronically excited molecular states: structure, reactivity, spectra (since 1958)
- Interstellar molecules: spectra, reactions (1990–2000)

Selected papers

1. Grabowski Z.R., Czochralska B., Vincenz-Chodkowska A. and Balasiewicz M.S., "Stereochemistry of electrode reactions", *Disc. Faraday Soc.*, **45**, 145–153; 178–9; 181 (1968).
2. Grabowski Z.R. and Rubaszewska W., "Generalized Förster cycle. Thermodynamic and extrathermodynamic relationships between proton transfer, electron transfer and electronic excitation", *J. Chem. Soc., Faraday Trans. I*, **73**, 11–28 (1977).
3. Grabowski Z.R., Rotkiewicz K., Siemiarczuk A., Cowley D.J. and Baumann W., "Twisted intramolecular charge transfer states (TICT). A new class of excited states with a full charge separation", *Nouv. J. Chim.*, **3**, 443–454 (1979).
4. Rullière C., Grabowski Z.R. and Dobkowski J., "Picosecond absorption spectra of carbonyl derivatives of dimethylaniline: the nature of the TICT excited states", *Chem. Phys. Lett.*, **137**, 408–413 (1987).
5. Karpiuk J., Grabowski Z.R. and DeSchryver F.C., "Photophysics of the lactone form of Rhodamin 101", *J. Phys. Chem.*, **98**, 3247–3256 (1994).
6. Kołos R. and Grabowski Z.R., "The chemistry and prospects for interstellar detection of some dicyanoacetylenes and other cyanoacetylene related species", *Astrophysics and Space Science*, **271**, 65–72 (2000)
7. Grabowski Z.R., Rotkiewicz K. and Rettig W., "Structural changes accompanying intramolecular electron transfer – focus on T.I.C.T. states and structures", Chemical Reviews, 103, 3899–4031 (2003).

Total number of publications: 115

Czesław Radzewicz, Professor



M.Sc., 1977 – Department of Physics, Warsaw University
Ph.D., 1984 – Department of Physics, Warsaw University
D.Sc., 1989 – Department of Physics, Warsaw University
Professor, 2000 – Department of Physics, Warsaw University

Education and training:

1983 – Department of Physics, University of Tubingen, Tubingen, Germany

1986-1987 – Institute of Optics, University of Rochester, Rochester, USA (research associate)

1991 - Institute of Optics, University of Rochester, Rochester, USA (Visiting Scientist)

1991-1992 – Department of Electrical and Computer Engineering, Oklahoma State University, Stillwater, USA (Visiting Professor)

1993 – Department of Physics, University of Crete, Irakion, Greece (Visiting Professor)

1996 – Department of Electrical and Computer Engineering, Oklahoma State University, Stillwater, USA (Visiting Professor

2002 – Department of Electrical and Computer Engineering, Oklahoma State University, Stillwater, USA (Visiting Professor)

Research areas:

- ultrafast laser science
- nonlinear and quantum optics
- femtosecond spectroscopy

Selected papers

1. Ratajska-Gadomska B., Gadomski W., Wiewiór P. and Radzewicz C., "Femtosecond snap-shot of crystaline order in molecular liquids", *J. Chem. Phys.*, **108**, 8489–8498 (1998).
2. Banaszek K., Radzewicz C., Wódkiewicz K. and Krasinski J.S., "Direct measurement of the Wigner function by photon counting", *Phys. Rev.*, **A60**, 674–677 (1999).
3. Banaszek K., Dragan A., Wódkiewicz K. and Radzewicz C., "Direct measurements of optical quasidistribution functions: Multimode theory and homodyne tests of Bell's inequalities", *Phys. Rev.*, **A66**, (2002).
4. Radzewicz C., Wasylczyk P., Wasilewski W. and Krasinski J.S., "Piezo-driven deformable mirror for femtosecond pulse shaping", *Opt. Lett.*, **29**, 177–179 (2004).
5. Płochocka P., Kossacki P., Maślana W. , Cibert J., Tatarenko S., Radzewicz C. and Gaj J., "Femtosecond study of the interplay between excitons, trions, and carriers in Cd1-xMnxTe quantum wells", *Phys. Rev. Lett.*, **92**, 177402 (2004).
6. Banaszek K., Dragan A., Wasilewski W. and Radzewicz C., "Experimental demonstration of entanglement-enhanced classical communication over a quantum channel with correlated noise", *Phys. Rev. Lett.*, **92**, 257901 (2004).
7. Wasylczyk P., Wasilewski W. and Radzewicz C., "A single-shot autocorrelator based on a Babinet compensator", *Rev. Scien. Instr.*, **75**, 2482 (2004).
8. Wojtkowski M., Bajraszewski T., Gorczyńska I., Targowski P., Wasilewski W., Kowalczyk A. and Radzewicz C., "Ophthalmic imaging by Spectral Optical Coherence Tomography", *American Journal of Ophthalmology*, **138**, 412–419 (2004).

Total numer of publications: 66

Krystyna Rotkiewicz, Professor

M.Sc., 1959 – Department of Chemistry, Technical University of Warsaw
Ph.D., 1968 – Institute of Physical Chemistry, Warsaw
D.Sc., 1990 – Institute of Physical Chemistry, Warsaw
Professor, 2001

Education and training:

Fellowship of Alexander von Humboldt Foundation
1970–1971 – Max-Planck Institute of Biophysical Chemistry, Göttingen, Germany
1977 – Institute of Physical Chemistry, University Mainz, Germany
1982/1983 – Institute of Organic Chemistry, Technical University, Aachen, Germany
1990 – Institute of Physical and Theoretical Chemistry, Technical University, Berlin, Germany

Professional affiliations:

- Polish Chemical Society
- European Photochemistry Association

Research areas:

- Intramolecular charge transfer processes in donor-aryl-acceptor compounds. Twisted Intramolecular Charge Transfer states, so-called TICT states
- Photochemical processes initiated by electron transfer step
- Photophysics and photochemistry in supramolecules

Selected papers

1. Rotkiewicz K., Grellmann K.-H. and Grabowski Z.R., "Reinterpretation of the Anomalous Fluorescence of p-N,N-dimethylaminobenzonitrile", *Chem. Phys. Lett.*, **19**, 315–318 (1973).
2. Rotkiewicz K., Grabowski Z.R. and Jasny J., "Picosecond Isomerisation Kinetics of Excited p-Dimethylaminobenzonitriles Studied by Oxygen Quenching of Fluorescence", *Chem. Phys. Lett.*, **34**, 55–59 (1973).
3. Rotkiewicz K. and Rubaszewska W., "Intramolecular Charge Transfer State and Unusual Fluorescence From an upper Excited Singlet of A Nonplanar Derivative of P-cyano-N,N-dimethylaniline", *J. Luminesc.*, **27**, 221–230 (1982).
4. Rotkiewicz K., Rechthaler K., Puchała A., Rasała D., Styrcz S. and Köhler G., "Dual Fluorescence and Intramolecular Charge Transfer in A Bulky Electron Donor-Acceptor System. N,N-dimethylaniline Substituted Bis-Pyrazolopiridine", *J. Photochem. Photobiol. A*, **98**, 15–19 (1996).
5. Okada T., Uesugi M., Köhler G., Rechthaler K., Rotkiewicz K., Rettig W. and Grabner G., "Time-Resolved Spectroscopy of Dmabn and Its Cage Derivatives – Cyanobenzquinuclidine (Cbq) and Benzquinuclidine (Bq)", *Chem. Phys.*, **241**, 327–337 (1999).
6. Miyasaka H., Itaya A., Rotkiewicz K. and Rechthaler K., "Picosecond Laser Photolysis Studies of Dma-Dmpp In Solution", *Chem. Phys. Lett.*, **307**, 121–130 (1999).
7. Grabner G., Rechthaler K., Mayer B., Köhler G. and Rotkiewicz K., "Solvent Influence on the Photophysics of Naphthalene. Fluorescence and Triplet State Properties in Aqueous Solutions and in Cyclodextrin Complexes", *J. Phys. Chem. A*, **104/7**, 1365–1376 (2000).
8. Othmen K., Boule P., Szczepanik B., Rotkiewicz K. and Grabner G., "Photochemistry of 4-Chloroaniline in Solution. Formation and Kinetic Properties of A New Carbene, 4-Imino-2,5-dienylidene", *J. Phys. Chem. A*, **104**, 9525–9534 (2000).

Total number of publications: 53, in press 2

Jerzy Herbich, Associate Professor

M.Sc., 1967 – Department of Chemistry, Technical University of Warsaw

Ph.D., 1977 – Institute of Physical Chemistry, Warsaw

D.Sc., 1998 – Institute of Physical Chemistry, Warsaw

Professional experience:

1978, 1982 – Rijksuniversiteit te Leiden, Huygens Laboratorium (Prof. J.H. van der Waals)

1988 – Universiteit te Amsterdam (Prof. R.P.H. Rettschnick)

1993 – Faculty of Science, Tohoku University, Sendai (Prof. T. Azumi)

1994, 1998, 1999, 2000, 2001 – Johann-Wolfgang-Goethe-Universität, Frankfurt am Main (Prof. B. Brutschy)

Professional affiliations:

- Polish Chemical Society (since 1968)
- European Photochemistry Association (elected member of EPA Standing Committee 1984–1986, 1986–1988, 1995–1997, 1997–1999, 2001–2003, 2003–2005)

Editorial affiliations:

- Member of the Editorial Board of European Photochemistry Association Newsletters

Research areas:

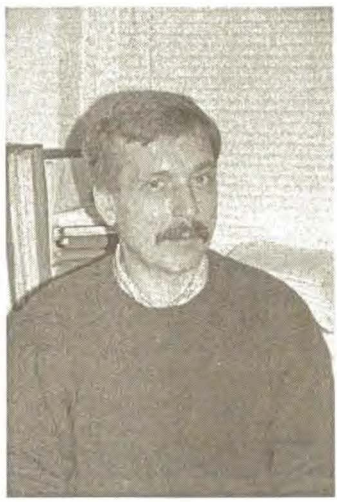
- Spectroscopy, photophysics and photochemistry of organic molecules. Structure and reactions of molecules in excited electronic states (especially: photoinduced electron transfer and photo-tautomerization processes)
- Electron spin resonance spectroscopy, laser spectroscopy and mass spectrometry combined with supersonic jet expansion technique

Selected papers

1. Herbich J., van Noort H.M., van der Poel W.A.J.A. and van der Waals J.H., "The triplet state of the quinoxalinium cation in a quinolinium perchlorate host crystal at 1.2 K", *Chem. Phys. Lett.*, **65**, 266–271 (1979).
2. Herbich J., Pérez-Salgado F., Rettschnick R.P.H., Grabowski Z.R. and Wójtowicz H., "Twisted intramolecular charge transfer state in supercooled molecules: structural effects and clustering with polar molecules", *J. Phys. Chem.*, **95**, 3491–3497 (1991).
3. Herbich J., Kapturkiewicz A. and Nowacki J., "Phosphorescent intramolecular charge transfer triplet states", *Chem. Phys. Lett.*, **262**, 633–642 (1996).
4. Herbich J., "Photoinduced intramolecular electron transfer in donor-acceptor molecules. Structural and environmental aspects", IChF PAN, Warszawa, pp. 1–169 (1998).
5. Kyrychenko A., Herbich J., Izydorzak M., Wu F., Thummel R.P. and Waluk J., "Role of ground state structure in photoinduced tautomerization in bifunctional proton donor-acceptor molecules: 1H-pyrrolo[3,2-h]quinoline and related compounds", *J. Am. Chem. Soc.*, **121**, 11179–11188 (1999).
6. Herbich J. and Brutschy B., "TICT molecules", in "Electron Transfer in Chemistry", V. Balzani, Ed., Wiley-VCH, Weinheim, 2001; Vol. 4, Section 3: "Gas Phase Systems", Chapter 3, pp. 697–741.
7. Herbich J., Kijak M., Zielińska A., Thummel R.P. and Waluk J., "Fluorescence Quenching by Pyridine and Derivatives Induced by Intermolecular Hydrogen Bonding to Pyrrole-Containing Heteroaromatics", *J. Phys. Chem. A*, **106**, 2158–2163 (2002).
8. Szydłowska I., Kubicki J. and Herbich J., "Picosecond kinetics of excited-state charge separation in 4-(dimethylamino)pyridine", *Photochem. Photobiol. Sci.*, **4**, 106–112 (2005)

Total number of publications: 70

Andrzej Kapturkiewicz, Associate Professor



M.Sc., 1977 – Department of Chemistry, University of Warsaw
Ph.D., 1984 – Institute of Physical Chemistry, Warsaw
D.Sc., 1993 – Institute of Physical Chemistry, Warsaw

Education and training:

1985–86 – Institute of Physical and Theoretical Chemistry, University of Erlangen, Germany (Fellowship of Alexander von Humboldt Foundation)
1989 – Institute of Chemical Physics AN USSR, Moscow, USSR
1991, 1994 – Institute of Physical and Theoretical Chemistry, University of Erlangen, Germany
1999, 2002 – Ecole Nationale Superieure de Chimie et Physique, University of Bordeaux, France
2000, 2003 – Institute of Physical and Theoretical Chemistry, Graz Technical University, Austria

Research area:

- Organic physical chemistry with special attention to kinetics of the electron transfer reaction studied by means of the electrochemical and spectroscopic techniques

Selected paper

1. Kapturkiewicz A., "Electron transfer and spin up-conversion processes", in *Electrogenerated Chemiluminescence*, Ch. 4, pp. 163–211, Edited by A.J. Bard, Marcell Dekker, New York (USA), (2004).
2. Kapturkiewicz A. and Angulo G., "Extremelly Efficient Electrochemiluminescence Systems Based on tris(2-phenylpyridine)-iridium(III)", *Dalton Trans.*, 3907 (2003).
3. Czerwieniec A., Kapturkiewicz A., Anulewicz-Ostrowska R. and Nowacki J., "Re(I)(tricarbonyl)$^+$ Complexes with the N O$^-$ Bidentate Ligands", *J. Chem. Soc. Dalton Trans.*, 3434 (2002).
4. Kapturkiewicz A., Szrebowaty P., Angulo G. and Grampp G.,. "Electron transfer quenching and electrochemiluminescence comparative studies of the system containing N-methylpyridinium cations and Ru(2,2′-bipyridine$_3^{2+}$ and Ru(1,10′-phenanthroline$_3^{2+}$ complexes", *J. Phys. Chem. A*, **106**, 1678 (2002).
5. Czerwieniec R., Kapturkiewicz A., Anulewicz-Ostrowska R. and Nowacki J., "Monomeric and dimeric Re(I)(tricarbonyl)(8-quinolinato) complexes", *J. Chem. Soc. Dalton Trans.*, 2756 (2001).
6. Szrebowaty P. and Kapturkierwicz A. "Free energy dependence on tris(2,2′-bipyridine)ruthenium(II) electrochemiluminescence efficiency", *Chem. Phys. Lett.*, **328**, 160 (2000).
7. Kapturkiewicz A. and Nowacki J., "Properties of the intramolecular excited charge-transfer states of carbazol-9-yl derivatives of aromatic ketones", *J. Phys. Chem. A.*, **103**, 8145 (1999).
8. Herbich J. and Kapturkiewicz A., "Electronic structure and molecular conformation in the excited charge transfer singlet states of p-acridyl and other aryl derivatives of aromatic amines", *J. Am. Chem. Soc.*, **120**, 1014 (1998).
9. Kapturkiewicz A., "Marcus theory in the qualitative and quantitative description of electrochemiluminescence phenomena". in *Advances in Electrochemical Science and Engineering*, Vol. 5, Ch. 1, pp. 1–60, Edited by R. Alkire, H. Gerischer, D.M. Kolb, C.W. Tobias, Wiley – VCH, Weinheim (Germany), 1997.
10. Herbich J., Kapturkiewicz A. and Nowacki J., "Phosphorescent intramolecular charge-transfer states" Chem. Phys. Lett., 262, 633 (1996).

Total number of publication: 47

Robert Kołos, Associate Professor

M.Sc., 1981 – Chemistry Department, University of Warsaw
Ph.D., 1991 – Institute of Physical Chemistry, Warsaw
Dr.Sc., 2003 – Institute of Physical Chemistry, Warsaw

Professional experience:

1981–1982 – Astronomical Observatory, Nicolaus Copernicus University, Toruń, Poland
1992–1993, 2004 – Laboratoire de Photophysique Moléculaire, Orsay, France
1999, 2000, 2001 – Eidgenössische Technische Hochschule, Zürich, Switzerland
2000 – Technische Universität München, Garching, Germany
2004 – Laboratoire Inter-Universitaire des Systemes Atmosphériques, Créteil, France
2005 – Université de Provence, Marseille, France

Professional affiliations:

- Polish Chemical Society

Main research areas:

- experimental astrochemistry
- molecular spectroscopy
- single molecule detection

Selected papers

1. Kołos R. and Dobrowolski J.Cz., "HCNCC – the possible isomer of cyanoacetylene", *Chem. Phys. Lett.*, **369**, 75–79 (2003).
2. Kołos R., "Exotic isomers of dicyanoacetylene: A density functional theory and ab initio study", *J. Chem. Phys.*, **117**, 2063–2067 (2002).
3. Sepioł J., Kołos R., Renn A. and Wild U.P., "Zero-phonon linewidths for single dibenzo-anthanthrene molecules in solid Xe", *Chem. Phys. Lett.*, **355**, 71–76 (2002).
4. Smith A.M., Lorenz M., Kołos R. and Bondybey V.E., "Vibrational spectra of matrix-isolated mass-selected cyanoacetylene cations", *J. Chem. Phys.*, **115**, 7534–7542 (2001).
5. Kołos R. and Sobolewski A.L., "The infrared spectroscopy of HNCCC: matrix isolation and density functional theory study". *Chem. Phys. Lett.*, **344**, 625–630 (2001).
6. Kołos R. and Grabowski Z.R. "The chemistry and prospects for interstellar detection of some dicyanoacetylenes and cyanoacetylene-related species"; *Astrophysics & Space Science*, **271**, 65–72 (2000).
7. Kołos R., "Photolysis of dicyanodiacetylene in argon matrices"; *Chem. Phys. Lett.*, **299/2**, 247–251 (1999).
8. Kołos R, Salloum A. and Dubost H., "Molecular hydrogen isotopomeres as traps of vibrational energy in low temperature matrices"; *Chem. Phys. Lett.*, **254**, 47–51 (1996).
9. Kołos R., "A novel source of transient species for matrix isolation studies"; *Chem. Phys. Lett.*, **247**, 289–292 (1995).
10. Kiszkurno E., Kołos R., Krełowski J. and Strobel A., "The distribution of the extinction in the Galactic disk"; *Astronomy & Astrophysics*, **351**, 337–340 (1984).
11. Kołos R. and Grabowski Z.R., "Chemical reactivity of the TICT states: unusual quenching by fluoride ion and by soft and hard bases"; *J. Mol. Struct.*, **84**, 251–258 (1982).

Total number of publications: 45

Marek Pietraszkiewicz, Associate Professor

M.Sc., 1973 – Department of Chemistry, Warsaw University
Ph.D., 1978 – Institute of Organic Chemistry, Warsaw;
D.Sci., 1992 – Institute of Organic Chemistry, Warsaw

Education and training:

1978–79 – post-doctoral position in Orleans University, France, prof. P. Sinay, works on the chiral synthesis of natural products from D-glucose
1982, 1984–85 – research associate in Universite Louis Pasteur de Strasbourg, France, prof. Jean-Marie Lehn, works on luminescent lanthanide complexes
1983, 85, 1990, 91 – six months at Sheffield University, UK, prof. J. Fraser Stoddart, works on crown ethers, rotaxanes and catenanes
1990, 91, 2 months, Odense University, Faculty of Chemistry, Denmark, Prof. Jan Becher, works on tetrathiafulvalene macrocycles

Administrative functions:

- Founder and Chairman of the Global Supramolecular Chemistry Network (GSCN)
- Executive Chairman of the Polish Supramolecular Chemistry Foundation (PSCNF)
- GSCN Regional Coordinator for Poland
- Chairman of the International Organizing Committee of the GSCN Supramolecular Science & Technology International Conferences
- Organizer of PSCNF Microsymposia in Poland
- more informations: http://www.gscn.org

Professional affiliations:

- Polish Chemical Society, since 1978
- European Rare Earth and Actinide Society, since 1990

Scientific interests:

supramolecular chemistry: molecular recognition, self-assembly and self-organization, calixarene chemistry, polyazamacrocycles and their transition metal complexes, macrocyclic luminescent lanthanide complexes, dendrimer chemistry, polyoxometalate hybrid materials, modified porphyrins synthesis, Langmuir films, sol-gel and xerogel organic/inorganic materials, composite functional multilayers.

Awards:

Award of the Scientific Secretary of the Polish Academy of Sciences, 1983 ; Award of the Third Division of the Polish Academy of Sciences, 1987.

Selected papers

1. Pietraszkiewicz M., Pietraszkiewicz O., Kołodziejski W., Woźniak K., Feeder N., Benevelli F. and Klinowski J., *J. Phys. Chem. B*, **104**, 1921 (2000).
2. Gawryszewska P., Jerzykiewicz L., Pietraszkiewicz M. and Legendziewicz J., *Richl. Inorg. Chem.*, **39**, 5365 (2000)
3. Zielińska D., Poels I., Pietraszkiewicz M., Radecki J., Geise H.J. and Nagels L.J., *J. of Chromatogr. A*, **915**, 25 (2001).
4. Luminescence of Europium(III) Compounds in Zirconia Xerogels, Reisfeld R., Saraidarov T., Pietraszkiewicz M. and Lis S., *Chem. Phys. Lett.*, **349**, 266 (2001).
5. Pietraszkiewicz M., Karpiuk J. and Staniszewski K., "Highly Luminescent Lanthanide Complexes based on Dendritic Phosphinoxides", *J. Alloys & Comp.*, **341**, 267 (2002).
6. Reisfeld R., Saraidarov T., Ziganski E., Gaft M., Lis S. and Pietraszkiewicz M., "Intensification of rare earths luminescence in glasses"; *J. Lumin.*, **102**, 243–247 (2003).
7. Klonkowski AM., Lis S., Pietraszkiewicz M., Hnatejko Z., Czarnobaj K. and Elbanowski M., "Luminescence properties of materials with of Eu(III) complexes: Role of ligand, coligant, anion, and matrix", *Chem. Mater.*, **15**, 656 (2003).

Total number of publications: above 110

Jerzy Sepioł, Associate Professor

M.Sc., 1971 – Department of Physics, University of Warsaw
Ph.D., 1977 – Department of Physics, University of Warsaw
D.Sc., 1995 – Institute of Physical Chemistry, Warsaw

Research areas:

- laser techniques and spectroscopy
- molecular spectroscopy (in: solutions, solids, supersonic jets)
- single molecules: microscopy and spectroscopy

Professional experience:

1978, 1985 – Max-Planck Institute fuer Biophysikalische Chemie

1980–81, 1986, 1992, 93....2001 – Laboratorium fuer Physikalische Chemie, ETH, Zurich

1990–91 – Laboratoire de Photophysique Moleculaire, CNRS UPR 3361

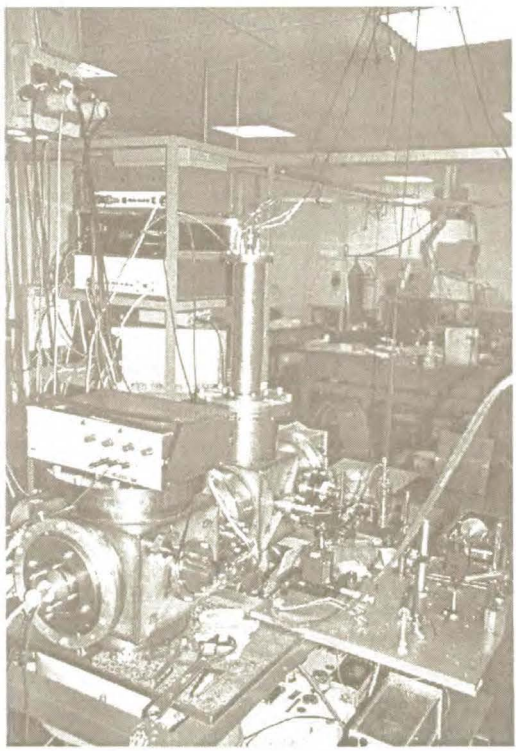
Selected papers

1. Sepioł J., "Stimulated Emission Pumping (Sep) As A Tool for Studying the Reversibility of the Excited-State Proton-Transfer Reaction of "Double"Benzoxazoles: 2,5-Bis(2-benzoxazolyl)Hydroquinone and 2,5-Bis(2-benzoxazolyl)-4-methoxyphenol" *Chem. Phys. Letters*, **175**, 419–424 (1990).
2. Lahmani F. and Sepioł J., "Spectral Hole-Burning Isolation of Fluorescent Species in Jet-Cooled 9-Methoxyanthracene Complexes with Water and Alcohols", *Chem. Phys. Letters*, **189**, 479–485 (1992).
3. Jasny J., Sepioł J., Irngartinger T., Traber M., Renn A. and Wild U.P., "Fluorescence Microscopy in Superfluid Helium: Single Molecule Imaging", *Rev. Sci. Instrum.*, **67**, 1425–1430 (1996).
4. Sepioł J., Jasny J., Keller J. and Wild U.P., "Single Molecules Observed by Immersion Mirror Objective. The Orientation of Terrylene Molecules..." *Chem.Phys. Letters*, **273**, 444–448 (1997).
5. Sepioł J., Stepanenko Y., Vdovin A., Mordziński A., Vogel E. and Waluk J., "Proton Tunnelling in Porphycene Seeded in A Supersonic Jet", *Chem. Pys. Letters*, **296**, 549–556 (1998).
6. Sepioł J., Starukhin A., Kołos R., Latychevskaia T., Jasny J., Renn A. and Wild U.P., "Detection and Spectroscopy of Single Molecules in Rare Gas Matrices: Dibenzanthanthrene in Krypton and Xenon", *Chem. Phys. Letters*, **311**, 29–35 (1999).

Total number of publications: 54

Laboratory of Molecular Beams

Head: Prof. Czesław Radzewicz

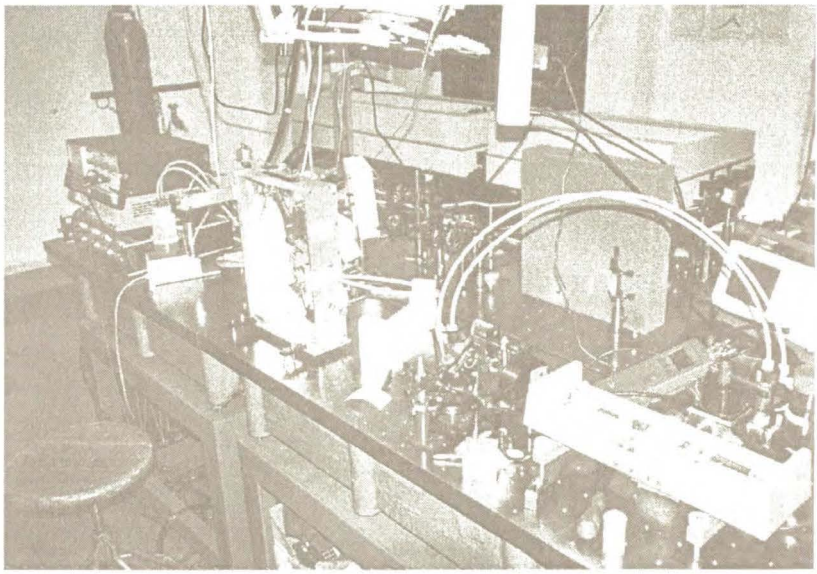


The research topics of this laboratory involve spectroscopy of chemical systems seeded in supersonic molecular beams. Supersonic expansion cools the vibrations and rotations of molecules without condensing out of the gas phase. In effect, the spectra of the molecules are greatly simplified. This allows us to probe the structure of isolated, supercooled large molecules in the gas phase, whose spectra are very complicated in other environments. Moreover, supersonic jets are an effective source to produce weakly bounded vdW and molecular complexes in the gas phase.

In our lab we utilize lasers to probe the structure, dynamics, vibrations of molecules and their molecular clusters. Our particular interests concern photoreactive molecules and chemical reactions of and in molecular clusters. These clusters are important models for understanding intermolecular interactions as well as structural, energetic and chemical features of solvents and solvation at a molecular level.

Example: R2PI (upper) and LIF excitation (lower) spectra of 3,3' dimethylene–2 (2' pyridyl)indole in supersonic jet.

A pulsed, tunable radiation from dye lasers and optical parametric oscillators are use for this purpose. Aromatic molecules and their molecular clusters are investigated by a variety of laser spectroscopy methods: laser induced fluorescence (LIF), dispersed emission, resonance two-photon ionization (R2PI), double-resonance population labeling ("hole burning"). The optical spectroscopy is usually completed with time-of-flight mass spectrometry to obtain mass-selective information.



Equipment:

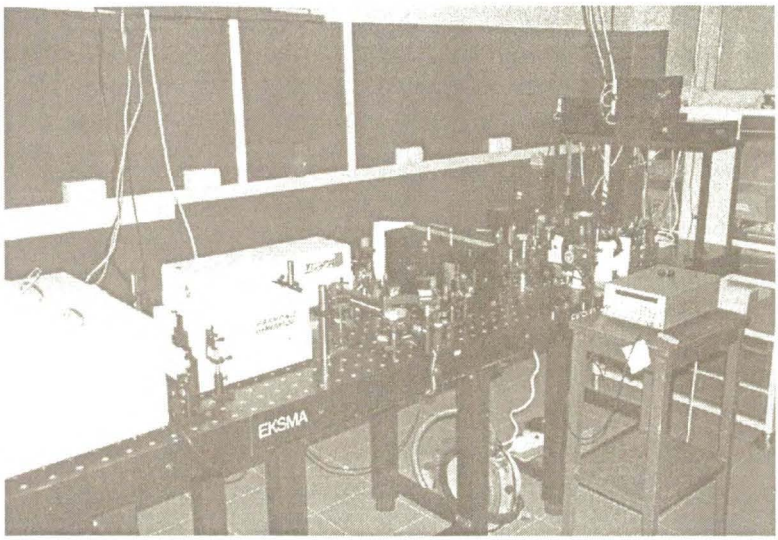
- 2 pulsed Nd:YAG lasers (10 Hz, 3–5 ns pulse width, 1064, 532, 355, 266 nm)
- 2 pulsed XeCl excimer lasers (10 Hz, 15–60 ns pulse width, 308 nm)
- 2 pulsed dye lasers (resolution 0.1–0.8 cm^{-1}, 340–850 nm)
- 1 optical parametric oscillator (resolution 0.08 cm^{-1}, 450–1650 nm)
- 2 systems (KDP, BBO) for generating tunable UV radiation by SHG
- 2 pulsed molecular beam setups including 0.5 m linear time-of-flight mass spectrometers and/or monochromators with PM and spectrograph with CCD camera

Contact persons:

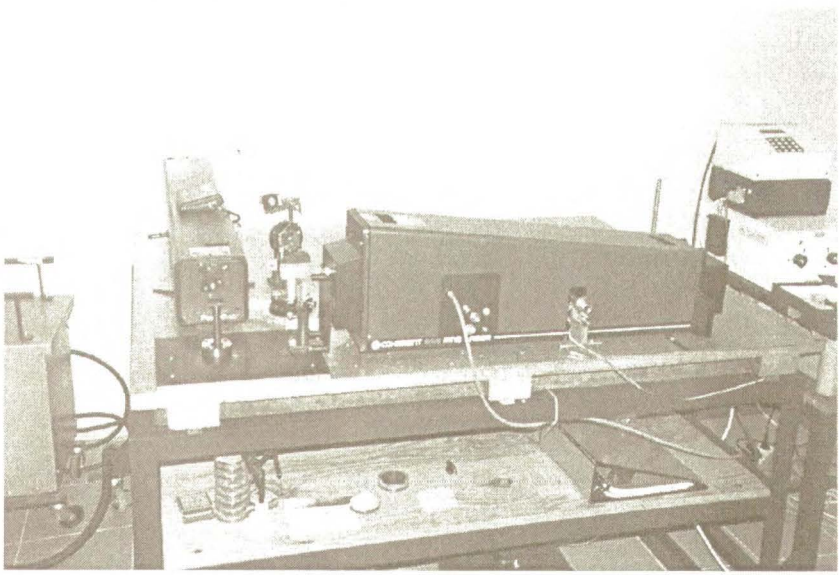
Prof. Czesław Radzewicz; radzewicz@fuw.edu.pl

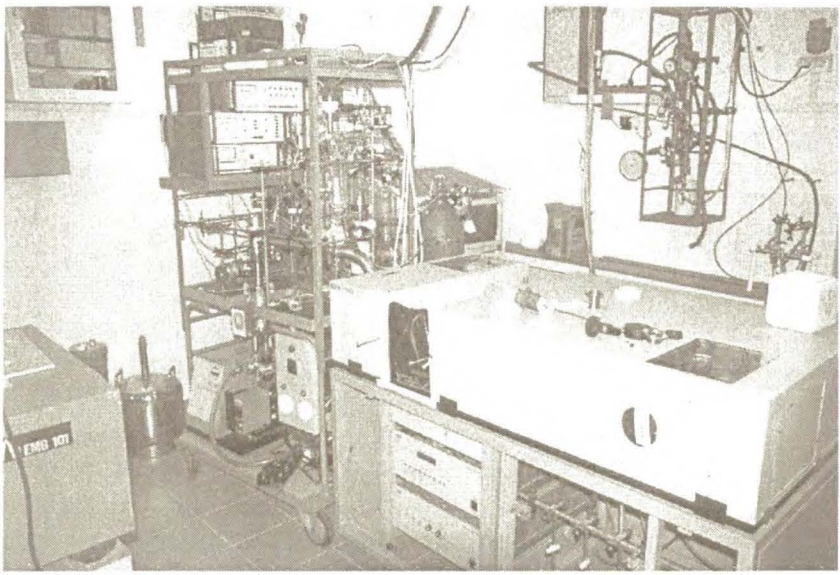
Laboratory of Spectroscopy and Photochemistry

Head: Prof. Jacek Waluk



We offer a variety of spectroscopic instruments and techniques that can be used in basic research as well as for analytical, kinetic, structural, environmental and industrial applications. Electronic and IR absorption, fluorescence and phosphorescence spectra can be measured in many different media (solutions, glasses, polymer films, crystals, powders, gas phase, cryogenic frozen gas matrices) at temperatures ranging from 4 K to about 500 K. Transient absorption/emission studies make it possible to detect the presence of reactive intermediates and to follow the kinetics of their formation and decay with time resolution spanning many orders of magnitude: from hours to a few picoseconds.





Photolysis of the samples is possible, applying intense and ultrashort laser pulses or high-power lamps. The photoproducts can be subsequently analysed by stationary and time-resolved optical techniques, as well as by electron spin resonance. Another way of generating transient species involves electrochemistry, coupled with electrochemiluminescence detection.

Polarized techniques used in both absorption and emission modes can provide information about transition moment directions, sample alignment and kinetic processes that are accompanied by spatial changes of the transition moments. We offer linear dichroism, magnetic circular dichroism and luminescence anisotropy measurements.

Our equipment includes three UV/VIS/IR spectrophotometers (Shimadzu and Cary), three lifetime and steady-state spectroflurimetric systems (Jasny and Edinburgh Instruments), numerous CW and pulsed lasers (argon, ring, dye, diode, excimer, nitrogen), high-intensity visible and UV lamps, picosecond transient absorption/emission setup (based on a Nd:glass 1 ps Light Conversion laser and a Topaz parametric oscillator), a gated/intensified CCD camera (S&I), an FTIR spectrometer (Nicolet SX 170), several closed-cycle and liquid helium cryostats, three matrix deposition lines, a home-built electrochemiluminescence spectrometer, an ESR spectrometer (JEOL). Many optical instruments have been custom-designed and built by Dr. Jan Jasny: those include, i.a., a unique nanosecond transient absorption spectrometer (–100 ns delay with a resolution of 1 ns, operation in the whole visible range), monochromators, several spectrographs with CCD or photodiode array detection, dye lasers, single-mode diode laser illuminator. The details can be found on our web page (http://malina.ichf.edu.pl/Dep9.html).

Contact persons:

Prof. Jacek Waluk
email:waluk@ichf.edu.pl

X. Department of Quantum Theory of Solids and Molecules

Head: Professor Andrzej Holas

The most interesting results in last years include:

- development of the density functional theory (DFT) foundations, in particular through the derivation of three different expressions for the exact exchange-correlation potential in the terms of density matrices, and through modification of the Hartree-Fock scheme by means of the perturbation expansion of density matrices, leading to the exact energy and electron density of the ground state of molecules;
- elaboration of a model describing dynamics of electrons in a magnetic field parallel to one of the crystallographic axes;
- calculations of structural and magnetic properties of metal surfaces and thin metallic layers using the tight-binding model.

At present, we are going to investigate an extension of the electron DFT to canonical ensembles with noninteger number of electrons, and to construct new approximate forms the of kinetic, exchange and correlation energy as functionals of the density, together with the corresponding potentials. We plan to perform modification of the Della Sala-Görling approximate exchange potential (which is used in DFT calculations of electronic structures) aiming at the improvement of its accuracy.

One of the new topics will be quantum-mechanical calculation of spin transport in magnetic nano-layers, with the help of methods worked out earlier for magnetic anisotropy calculations. Worth mentioning are also NMR studies (planned in cooperation with partners from outside of the Institute) of cyclodextrin complexes, and quantum chemical calculations of: (a) supramolecular systems, (b) chemical shifts and coupling constants in NMR spectra (sometimes accompanied by measurements), and (c) quantum calculations of hydrocarbons with unusual spatial structure with the aim to propose plausible synthetic targets.

It should be mentioned that the Department cooperates with several foreign centres: Imperial College, London (Prof. D.M. Edwards), Open University in Milton Keynes, UK, (Dr A. Umerski), Brussels Open University (Prof. P. Geerlings), University of Antwerp (Prof. N.H. March), Jackson State University, Miss., USA (Prof. J. Leszczyński).

Andrzej Holas, Professor

M.Sc., 1964 – Department of Mathematics and Physics, University of Warsaw
Ph.D., 1970 – Moscow Engineering and Physics Institute, USSR
D.Sc., 1981 – Institute of Nuclear Research, Warsaw-Świerk
Professor, 1997 – Institute of Physical Chemistry, Warsaw

Education and training:

1966–70, 1974–77 – Joint Institute for Nuclear Research, Dubna, USSR
1978–80 – Northwestern University, Evanston, IL, USA
1984–2001 – International Centre for Theoretical Physics, Trieste, Italy (one or two months each year)
1994, 1996 – University of Oxford, UK

Professional affiliations:

- American Physical Society

Research areas:

- Density-functional theory of many-electron systems
- Many-body theory approach to a homogeneous electron liquid
- Theory of normal metals properties

Selected papers

1. Brovman E.G., Kagan Yu. and Holas A., "Properties of the Metallic Hydrogen under Pressure", *Zh. Eksp. Teor. Fiz.*, **62**, 1492–1501 (1972); [**Sov. Phys. JETP**, **35**, 783–787 (1972)].
2. Holas A., Aravind P.K. and Singwi K.S., "Dynamic Correlations in an Electron Gas: I. First Order Perturbation Theory", *Phys. Rev. B*, **20**, 4912–4934 (1979).
3. Holas A., "Exact Asymptotic Expression for the Static Dielectric Function of a Uniform Electron Liquid at Large Wave Vectors", in "Strongly Coupled Plasma Physics", (Rogers F.J., Dewitt H.E., Eds.) NATO ASI Ser. B, Vol. 154, Plenum Press, New York 1987, pp. 463–482; [another version in "Electronic Structure of Solids" (Ziesche P., Ed.), Nova Science Publ., New York 1991, pp. 61–66].
4. Holas A. and March N.H., "Exact Exchange-Correlation Potential, and Approximate Exchange Potential, in Terms of Density Matrices", *Phys. Rev. A*, **51**, 2040–2048 (1995).
5. Holas A. and March N.H., "Exchange and Correlation in Density Functional Theory of Atoms and Molecules", in "Topics in Current Chemistry, Vol. 180", (Nalewajski R.F., Ed.), Springer-Verlag, Heidelberg, 1996, pp. 57–106.
6. Holas A., "Exact Modified-Hartree-Fock Scheme Through Perturbation Expansion of Density Matrices", *Int. J. Quantum Chem.*, **69**, 469–483 (1998).
7. Holas A. and March N.H., "Field Dependence of the Energy of a Molecule in a Magnetic Field", *Phys. Rev. A*, **60**, 2853–2866 (1999).

Total number of publications: 89

Helena Dodziuk, Professor

M. Sc., 1964 – Department of Physics, University of Warsaw
Ph.D., 1972 – Institute of Organic Chemistry, Warsaw
D.Sc., 1991 – Department of Mathematics, Physics and Chemistry, University of Wrocław

Education and training:

1967 – INEOS, Moscow, USSR
1973 – ETH, Zürich, 11 Switzerland
1980 – University of Georgia, Athens, Georgia, USA
1989 – 1990 - IUPUI, Indianapolis, USA.

Research areas:

- Stereochemistry
- Molecular modelling
- Supramolecular chemistry
- Hydrocarbons with nonstandard spatial structure
- Cyclodextrins
- Fullerenes
- Nanotubes

Selected publications

Books:

1. Dodziuk H., "*Modern Conformational Analysis. Elucidating Novel Exciting Molecular Structures*", VCH Publishers, NY, 1995.
2. Dodziuk H., "Introduction to Supramolecular Chemistry", Kluver, Dordrecht, 2002.

Articles:

1. Dodziuk H., "Unusual saturated hydrocarbons : interaction between theoretical and synthetic chemistry", *Top. Stereochem.*, **21**, 351 (1994).
2. Dodziuk H., Leszczyński J. and Nowiński K., "In quest for planar and pyramidal carbon atom. Can a tetrahedrally coordinated carbon form a nearly linear C-C-C bond angle?", *J. Org. Chem.*, **60**, 860 (1995).
3. Dodziuk H. and Nowiński K., "Horror vacui or topological in-out isomerism in perhydrogenated fullerenes. $C_{60}H_{60}$ and monoalkylated perhydrogenated fullerenes", *Chem. Phys. Lett.*, **249**, 406 (1996).
4. Dodziuk H., Ejchart A., Lukin O. and Vysotsky M.O., "^{1}H and ^{13}C NMR and Molecular Dynamics Study of Chiral Recognition of Camphor Enantiomers by α-Cyclodextrin", *J. Org. Chem.*, **64**, 1503 (1999).
5. Dodziuk H., Leszczyński J. and Jackowski K., "Small-ring geminanes – new hypothetical molecules with inverted carbon atoms", *J. Org. Chem.*, **64**, 6177 (1999).
6. Dodziuk H. and Lukin O., "The dependence of the average energy difference for the diastereomeric complexes of α-pinene enantiomers with α-cyclodextrin on the length of dynamic simulations", *Chem. Phys. Lett.*, **327**, 18 (2000).

Total number of publications: 70

Stanisław Olszewski, Professor Emeritus

M.Sc., 1954 – Department of Physics, University of Warsaw
Chem. Eng., 1954 – Technical University of Warsaw
Ph.D., 1962 – University of Paris, Centre Orsay, France
D.Sc., 1964 – Institute of Physical Chemistry, Warsaw
Professor, 1971 – Institute of Physical Chemistry, Warsaw

Education and training:

1957 – Technical University of Budapest, Hungary
1959–60 – University of Paris. Centre Orsay, France
1961–62 – University of Paris. Centre Orsay, France
1967–68 – Imperial College of Science and Technology, University of London, England
1982 – Joseph-Fourier University of Grenoble, France (visiting professor)
1988 – University of Paris-Sud, France (visiting professor)
1989 – Joseph-Fourier University of Grenoble, France (visiting professor)
1993, 1994 – Universitaire Instelling Antwerpen, Wilrijk, Antwerpen, Belgium

Professional affiliations:

- Polish Chemical Society
- Polish Physical Society
- European Academy of Sciences and Arts

Research areas:

Applications of quantum mechanics, especially to many-electron systems in solids and molecules:

- Free-electron gas method applied to polyenes and cyanine dyes
- Extension of the self-consistent equations by the correlation potentials
- Non-Bloch approach to the tight-binding method for the band structure of solids
- Extension of the Thomas-Fermi-Dirac method applied to the crystal structure of ionic compounds
- Time-scale problem from the point of view of the quantum-mechanical perturbation theory
- Dynamics of metal electrons in magnetic field

Selected papers

1. Olszewski S., "Remark on the theory of absorption spectra of symmetrical cyanine dyes and polyenes", *J. Chem. Phys.*, **26**, 1205–1207 (1957).
2. Olszewski S., "Simplified self-consistent field equations with correlations", *Phys. Rev.*, **121**, 42–45 (1961).
3. Olszewski S., "New approach to the linear-combination-of-atomic-orbitals method for cubic crystals", *Phys. Rev. B*, **3**, 4361–4377 (1971).
4. Modrak P. and Olszewski S., "Non-Bloch electron states in perfect cubic crystals" *Phys. Rev. B*, **14**, 2387–2397 (1976).
5. Kucharczyk M. and Olszewski S., "Effect of the local exchange-correlation correction to electron density on properties of inorganic solids", *J. Chem. Phys.*, **74**, 6319–6341 (1981).
6. Olszewski S., "Time scale and its application in perturbation theory", *Z. Naturforsch.*, **46a**, 313–320 (1991).
7. Olszewski S., Roliński T. and Kwiatkowski., "Fourier analysis applied to cyclotron resonance in metals having anisotropic Fermi Surfaces", *Phys.Rev. B*, 3740–3768 (1999).

Total number of publications: 103

Specialized Laboratories

Name Index