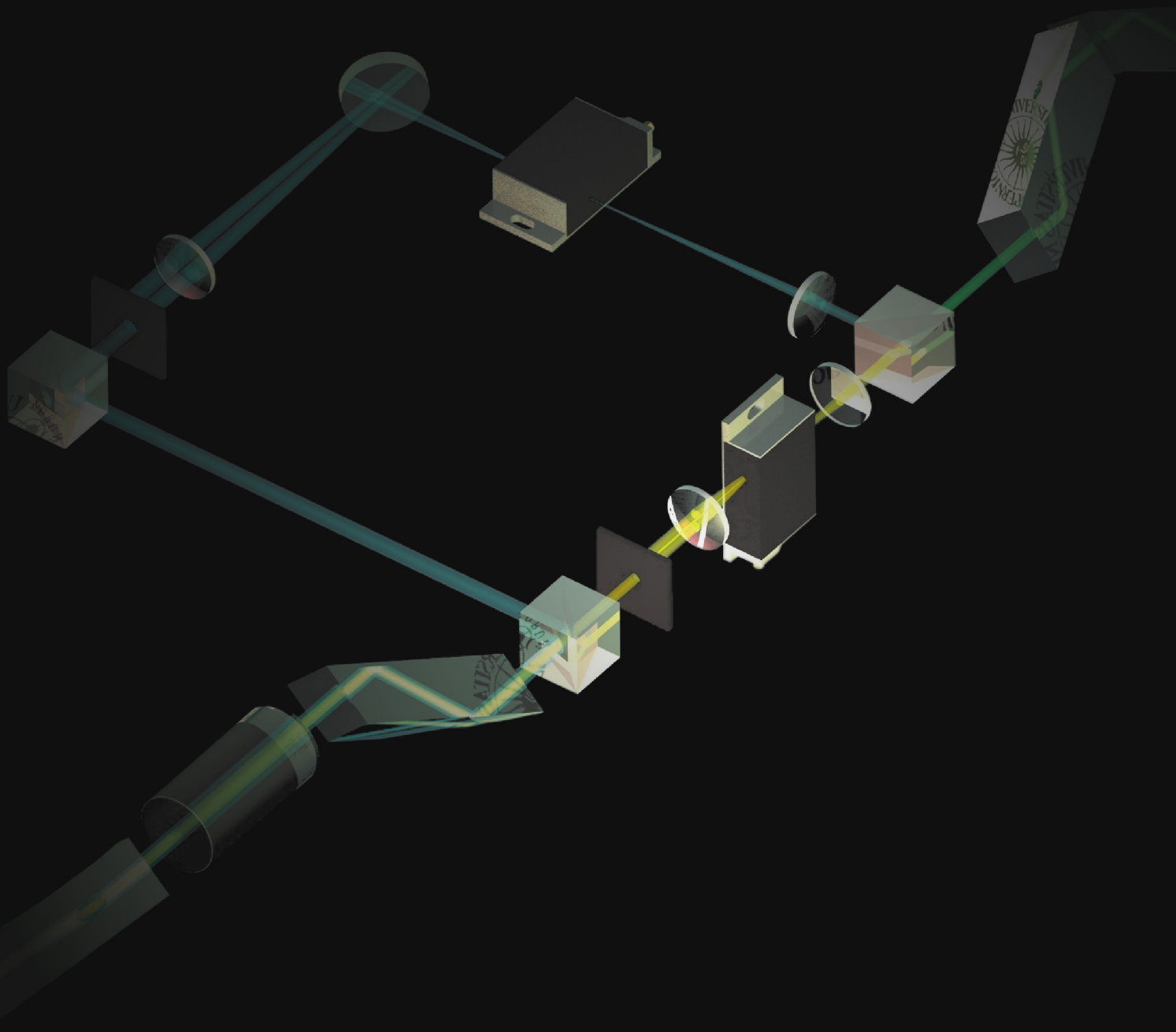


Physics at Nicolaus Copernicus University



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On the cover:

Electromagnetically induced transparency system
for the light storing (FAMO Lab)

Physics at Nicolaus Copernicus University



Institute of Physics

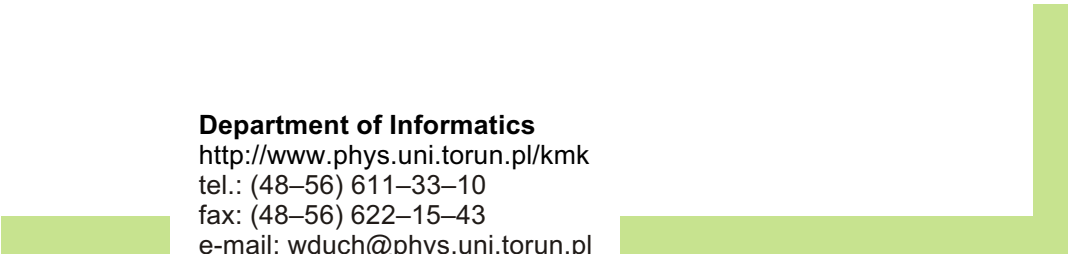
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Historically, **Toruń** is one of the most important cities in Poland. It also is one of the most attractive and best preserved. Having survived centuries of wars and conflicts the city offers a wealth of architectural treasures. In 1997 Toruń was included in the UNESCO World Heritage List.



This booklet is a report on the physics research at Nicolaus Copernicus University. It covers the activity of three units. Two of them: the Institute of Physics and the Department of Informatics are regular parts of the Faculty of Physics, Astronomy and Informatics. The third one, the National Laboratory for Atomic, Molecular and Optical Physics was founded in 2002 as a national facility open to researchers of the whole Country. The booklet presents the research interests rather than the results. The updated information about the projects, results, publications, researchers etc. can be found in our WWW pages <http://www.phys.uni.torun.pl>

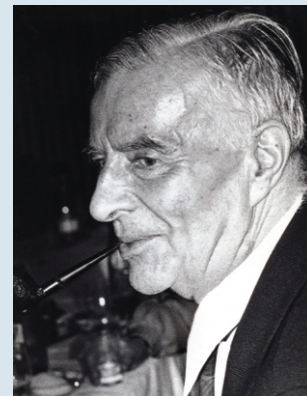
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Physics in Toruń

History

Nicolaus Copernicus University in Toruń was founded in the fall of 1945. On January 1, 1946, Aleksander Jabłoński (1898–1980) was appointed full professor of experimental physics of the University and charged with the task of organizing its Department of Physics. Working in the very difficult postwar years, in a country totally destroyed by World War II, he was able to establish here, as early as the beginning of the 1950's, a scientific center for experimental and theoretical studies in atomic and molecular physics, in particular, in his own fields of research on luminescence of liquids, gases and solids as well as pressure effects on spectral lines. This center consisted at that time of the Department of Physics of Nicolaus Copernicus University and the Laboratory for Photoluminescence of the Polish Academy of Sciences. It was located in *Collegium Physicum* — an University building completed in 1951 at Grudziądzka street. In the beginning the Department of Physics consisted of two Chairs: Experimental and Theoretical Physics. Holding the Chair of Experimental Physics, Jabłoński also contributed to initiating research in other fields, such as solid state physics and, in the following years, quantum electronics and molecular biophysics.



Aleksander Jabłoński



Apolonia Wrzesińska



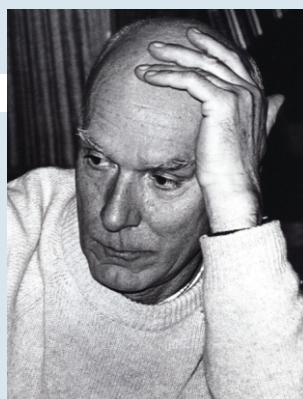
Kazimierz Antonowicz

Research in the field of solid state physics began in 1951 when Apolonia Wrzesińska (1910–1997) started her studies on photoluminescence and thermoluminescence phenomena in solids.

In 1956, Kazimierz Antonowicz (1914–2002) initiated his pioneering experiments in nuclear magnetic resonance (NMR). Later, he applied successfully radiospectroscopic techniques to the study of the properties of carbon materials.



Jerzy Rayski



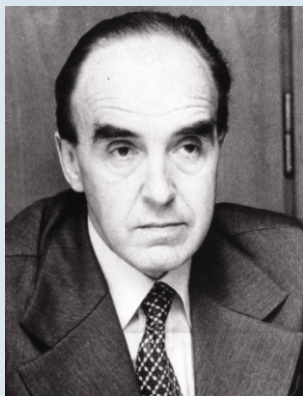
Jan Rzewuski



Wanda Hanus

Two Professors of theoretical physics: Jerzy Rayski (1917–1994; the Chair in 1947–1957) and Jan Rzewuski (1916–1994), who achieved widely acclaimed results in quantum field theory and in the theory of elementary particles, played an important role in the development of physics at Nicolaus Copernicus University. Rzewuski left Toruń in 1953 when he accepted the chair of theoretical physics at the University of Wrocław. In 1957 Rayski moved to Cracow where he was appointed professor of theoretical physics at the Jagellonian University. Rayski's successor to the Chair of Theoretical Physics of Nicolaus Copernicus University till 1969 was Wanda Hanus (1914–1973). Her research work was devoted to the theory of atomic spectra and relativistic quantum mechanics.

In 1958, Wiesław Woźnicki (1933–1995) joined the Theoretical Physics Chair. He came from Warsaw just after he had got the Ph. D. degree under Leopold Infeld. In early 1960s he gathered several young researchers who formed an informal group interested in chemical physics and quantum chemistry. In 1970's and 1980's the group was very strong as the Department of Chemical Physics headed by Professor Woźnicki. Several Departments working nowadays have originated from that one.



Wiesław Woźnicki

In 1991, Brian G. Wybourne (1935–2003) from the University of Canterbury in Christchurch, New Zealand joined our faculty. He spent in Toruń his last twelve years working on applications of symmetry in physics. He strongly influenced the development of the scientific community in Toruń.



Brian G. Wybourne

In 1966, Professor Roman S. Ingarden (presently retired, *Doctor Honoris Causa* of Nicolaus Copernicus University) came from Wrocław to Toruń to take the newly created Chair of Thermodynamics and Theory of Radiation. In Toruń he developed research in the field of mathematical physics, in particular on the foundations of statistical physics. He has had a great influence on the further development of physical sciences in Toruń.

In the middle 1960's, the Department of Physics of Copernicus University consisted of four Chairs: Experimental Physics (A. Jabłoński), Electronics and Solid State Physics (K. Antonowicz), Theoretical Physics (W. Hanus), and Thermodynamics and Theory of Radiation (R. S. Ingarden). Professor Jabłoński was the head of the Department from its beginning in 1946 until his retirement in 1968.

In 1969, the structures of University faculties were reorganized: institutes — units coordinating the scientific and educational activities of various research groups — were founded. The Department of Physics was replaced by the Institute of Physics. The first Director of the Institute was Roman Ingarden (from 1969 until 1978). In the following years, this post was held successively by Ryszard Bauer (1978–1981), Lutosław Wolniewicz (1981–1983), Józef S. Kwiatkowski (1984), and Józef Szudy (1984–2002). Currently, Stanisław Chwirot is the director.

Nowadays

Now, the **Institute of Physics** consists of eight research departments and of Education of Physics Laboratory. The Institute is a part of the Faculty of Physics, Astronomy and Informatics. Another part of the Faculty is the **Department of Informatics**. It arose in 1991 from the Institute and now is independent of it. Nevertheless, its research activity apart from informatics is also physics, especially

computational methods of physics. In 2002 another physics research unit was established in Toruń: **National Laboratory for Atomic, Molecular and Optical Physics**. It offers great experimental equipment and it is open via a grant system to all researchers of Poland.

All these three units are located in the University building known for many years as *Collegium Physicum* at Grudziądzka street. In 1980, after the death of Professor Jabłoński, that name was replaced by the *Aleksander Jabłoński Institute*.



Department of Atomic, Molecular and Optical Physics

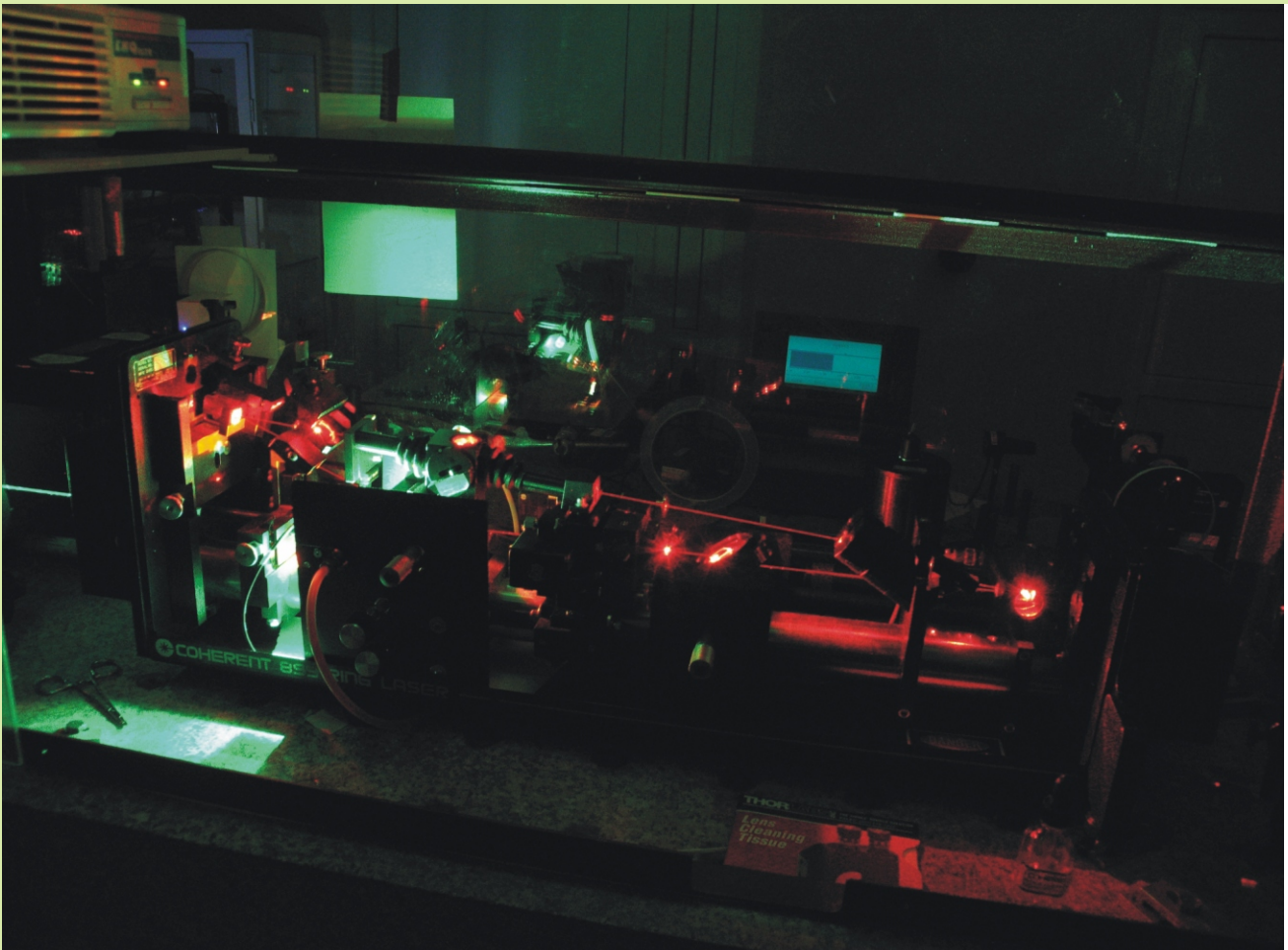
Head: Prof. dr hab. Józef Szudy

Prof. dr hab. Andrzej Bielski
Prof. dr hab. Stanisław Chwirot
Doc. dr hab. Franciszek Bylicki
Dr hab. Felicja Mrugała
Dr hab. Tadeusz Orlikowski
Dr hab. Piotr Rudecki
Dr hab. Ryszard S. Trawiński
Dr Konrad Banaszek
Dr Roman Ciuryło
Dr Jolanta Domysławska
Dr Dariusz Dżiczek
Dr Daniel Lisak
Dr Mariusz Piwiński
Dr Jerzy Wolnikowski
Wiktor Brączkowski

Ph. D. students:

Piotr Masłowski, M. Sc.
Łukasz Kłosowski, M. Sc. eng.

The Department is composed of three research groups.



High Resolution Spectroscopy Group

Andrzej Bielski – head of the group, Józef Szudy, Franciszek Bylicki, Ryszard S. Trawiński, Piotr Rudecki, Roman Ciuryło, Jolanta Domysławska, Daniel Lisak, Jerzy Wolnikowski, Piotr Masłowski

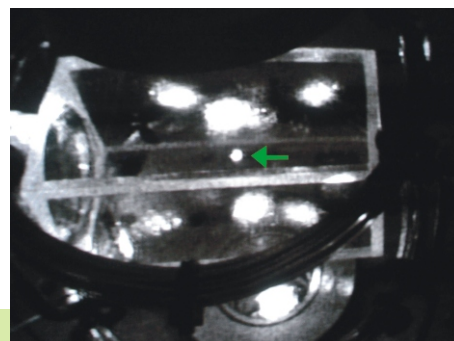
High resolution spectroscopy methods are used to gain a better understanding of the mechanisms of optical collisions in the gas phase resulting from the interatomic and intermolecular interactions involving excited states. Main attention is focused on both experimental and theoretical studies of pressure broadening, shift and asymmetry of atomic spectral lines perturbed by neutral particles such as ground-state atoms or molecules. Laser-induced fluorescence (LIF) technique as well as pressure-scanned Fabry-Perot interferometers are used to determine more subtle features of spectral line shapes in dilute gases. These features include: speed-dependent effects, correlation between velocity-changing and dephasing collisions as well as effects due to the finite duration of collisions.

Using a LIF method precise measurements of pressure-broadened profiles of the 326.1 nm intercombination line ($5^1S_0 - 5^3P_1$) of the even-even ^{114}Cd isotope perturbed by all rare gases and some molecular gases (H_2 , D_2 , N_2 and CH_4) were performed at pressures up to 600 Torr. The line shapes were analyzed in terms of a Speed-Dependent Asymmetric Voigt Profile (SDAVP) and the role of the correlation between pressure broadening rate and emitter velocity as well as of the finite duration of collisions were thoroughly investigated. The velocity-changing collisions were described by the billiard-ball (BB) model, which allows us to capture the dependence of velocity-changing collisions on the ratio α of the mass of perturber to emitter. For Cd-Xe ($\alpha=1.15$) we have observed that the Doppler width of the 326.1 nm Cd line obtained from the fit of the measured profile to the ordinary Voigt profile is significantly smaller than the value corresponding to the cell temperature. To verify the reason for this narrowing we have used an Asymmetric Billiard-Ball Profile (ABBP) as well as Speed-Dependent ABBP in which Dicke narrowing is taken into account using the BB model. The Dicke narrowing itself cannot completely eliminate departures between the fitted BB and experimental profiles. Contrary to that the use of SDAVP, which takes into account correlation between pressure and Doppler broadening but neglects Dicke narrowing, gives rise to residuals which are spread uniformly about zero. Good quality of SDAVP fit indicates that narrowing of atomic lines is really dominated by speed dependence of pressure broadening and shift rates and the role of Dicke narrowing is diminished in the optical domain.

Other topics of interest deal with:

1. Determination of total cross-sections for impact broadening and shift of the 326.1 nm ^{114}Cd line perturbed by various atomic and molecular perturbers;
2. Line-mixing asymmetry in profiles associated with the hyper-fine-structure components of the intercombination transition ($5^1S_0 - 5^3P_1$) of the even-odd ^{113}Cd isotope;
3. Influence of velocity-changing collisions (Dicke narrowing) and line mixing on infrared molecular lines in the $03^1_0 \leftarrow 01^1_0$ Q branch of N_2O (*in collaboration with the group of J.D. Drummond and A.D. May at University of Toronto, Canada*);
4. Pressure broadening and shift of H_2O and C_2H_2 lines in the region around 3 μm (*in collaboration with the group of A. Sasso at Universita di Napoli, Italy*);
5. Properties of photoassociation spectra near the intercombination line (the weak transition between 1S_0 and 3P_1 states) of cold alkaline earth atoms; calculations have been carried out for calcium atoms colliding at ultra low temperatures of 1mK, 1 μK and 1 nK (*in collaboration with the group of Paul S. Julienne at National Institute of Standards and Technology, Gaithersburg, MD, USA*);
6. At the end of 2004 a magneto-optical trap (MOT) was built. In the near future it will be used to study the properties of cold Rb atoms at temperatures of about 100 μK .

Torunian MOT



Fundamental Atomic Interactions Group

Stanisław Chwirot – head of the group, Konrad Banaszek, Dariusz Dziczek, Mariusz Piwiński, Łukasz Kłosowski

Sophisticated experimental methods are used to study some of the fundamental interactions of atoms. Special techniques are applied to limit the extent of averaging over experimental parameters and provide data which characterize researched phenomena at the level as close to single interaction event as possible.

Present scope of interest of the group include:

1. Electron impact excitation of atoms

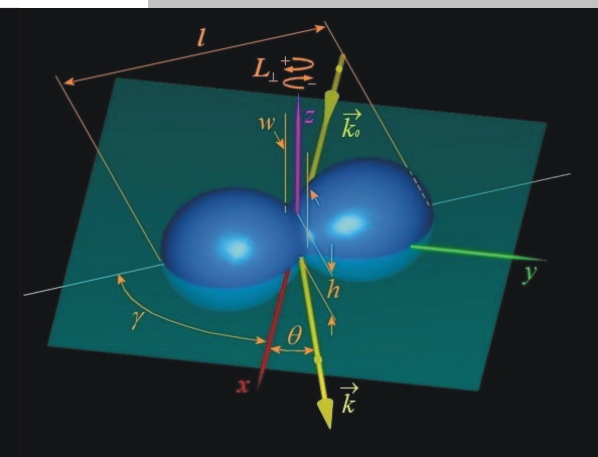
- electron-photon coincidence technique is used to acquire data on *electron impact coherence parameters (EICP)* which characterize properties (the shape and spatial orientation) of the electron cloud of the excited atom immediately after the collision with electron (currently, $4^1S_1 - 5^1P_1$ excitation of cadmium atoms is studied),
- measurements of *optical excitation functions* (dependence of excitation cross section on electron energy) and *polarization functions* (energy dependence of polarization of electron impact-induced fluorescence);

2. Coherent interactions of atoms with multiple radiation fields —

- atomic media in the state of *Coherent Population Trapping (CPT)*
- propagation of light pulses with electromagnetically-controlled group velocity,
- “light storage” – suspension of propagation of light pulses in atomic media;

3. Entangled photons and quantum information processing

- generation of tailored single-photon wave packets in non-linear media,
- protecting coherent superposition states in quantum communication.



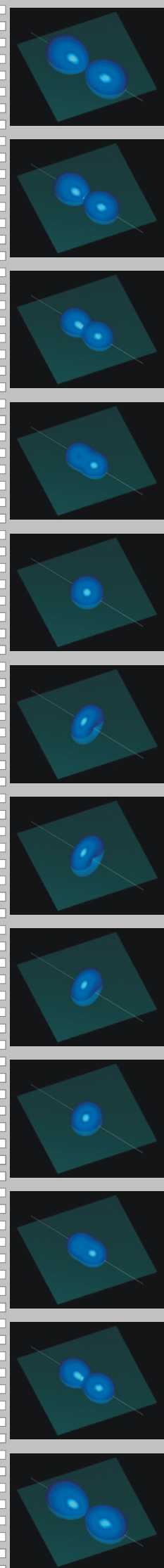
Graphical representation of angular distribution of electron cloud of a collisionally excited atom. The indicated parameters can be determined in electron – photon coincidence experiments.

Molecular Collision Theory Group

Tadeusz Orlikowski – head of the group, Felicja Mrugała

The research of the group concerns the methodological and applicative aspects of collision theory. Of particular interest are methods for accurate quantum-mechanical (*close-coupling*) calculations on collision and half-collision processes in small molecular systems. Invariant imbedding-type algorithms for evaluation of various detailed characteristics of the processes and computer programs elaborated in our group are currently used in studies of the following problems:

- 1. Collisions of open-shell atoms and diatomic molecules** (polarization effects).
- 2. Low-energy atomic collisions.**
- 3. Collisional broadening of spectral lines.**
- 4. Dynamics and spectroscopy of atom-diatom van der Waals molecules** (rotational and vibrational predissociation effects).
- 5. Radiative association and radiative charge transfer reactions** in collisions of helium ions with hydrogen molecules at low temperatures (first rigorous state-to-state study of the reactions in a triatomic system).



Department of Quantum Physics

Head: Prof. dr hab. Jarosław Zaremba

Prof. dr hab. Stanisław Dembiński
 Prof. dr hab. Włodzimierz Jaskólski
 Prof. dr hab. Jacek Karwowski
 Prof. dr hab. Adam J. Makowski
 Prof. dr hab. Andrzej Raczyński
 Prof. dr hab. Lutosław Wolniewicz (emeritus)
 Dr hab. Grażyna Staszewska, prof. UMK*
 Dr hab. Mirosław Bylicki, prof. UMK
 Dr hab. Jan Iwaniszewski
 Dr hab. Jacek Kobus
 Dr hab. Piotr Peplowski
 Dr hab. Lidia Smentek**
 Dr Dorota Bielińska-Wąż
 Dr Jacek Matulewski
 Dr Rafał Oszwałdowski
 Dr Grzegorz Pestka
 Dr Monika Stanke

Ph. D. students:

Lech Cyrnek, M. Sc.
 Katarzyna Górka, M. Sc.
 Andrzej Kędziorski, M. Sc.
 Piotr Matuszak, M. Sc.
 Małgorzata Rzepecka, M. Sc.
 Artur Stachów, M. Sc.
 Piotr Weber, M.Sc.
 Aleksander Wozinski, M. Sc.
 Tomasz Zakrzewski, M. Sc.
 Michał Zieliński, M. Sc.
 Krzysztof Żebrowski, M. Sc.

General research directions include: foundations of quantum mechanics, applications of quantum mechanics to modeling many-electron systems, quantum optics, atomic and molecular spectroscopy, theory of nano-structures, theory of open systems.

The Department is composed of seven Research Groups:

Applied Quantum Mechanics Group

Grażyna Staszewska – head of the group, Lutosław Wolniewicz, Krzysztof Żebrowski

Research areas:

1. Investigations of the spectroscopic properties of two-electron molecules

Theoretical ab initio studies of various spectroscopic properties of excited states of the hydrogen molecule and its isotopomers including adiabatic, non-adiabatic and relativistic effects are performed.

Methods allowing to achieve accuracy comparable with experimental data are developed.

2. Theoretical description of nanoenergetic materials

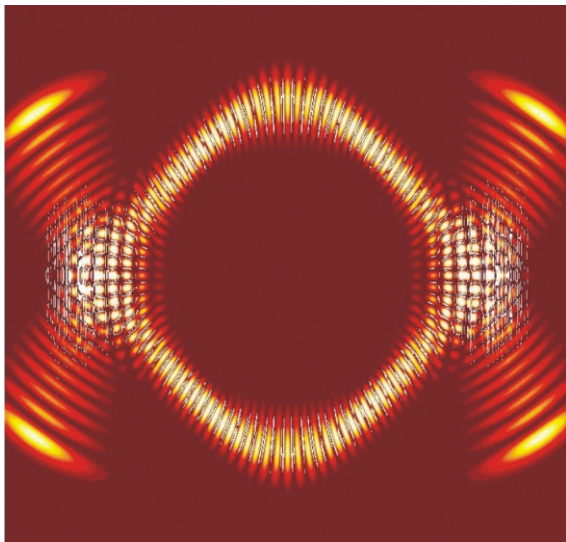
The methods for characterizing the structure and energetic properties of nanoparticles are developed. This includes the modeling the potential energy surfaces for nanoparticles composed of aluminium and hydrocarbons as well as performing dynamics calculations.

3. The study of the optical potential method for electron-atom scattering

The effective polarization and absorption, energy dependent, local potentials for electron scattering are modeled. Quasifree-scattering model for absorption potential and its recent modifications are investigated and new parametrizations of the effective potentials are studied.

* UMK is the abbreviation from Uniwersytet Mikołaja Kopernika.

**Also a Professor of Chemistry at Vanderbilt University, Nashville, TN, USA.



The probability density of a coherent state localized on classical Lissajous figures

Foundations of Quantum Mechanics Group

Adam J. Makowski – head of the group, Katarzyna Górska

We are interested in two complementary processes: how to quantize an initially classical system and how to recover the classical world from the quantum physics. Basically this implies studying the interrelations between the classical and quantum ways of thinking. These include: various methods of quantization, the problems of taking the limits of the Planck constant approaching zero and high quantum numbers, Ehrenfest's-like equations, the phase-space formulations, the quantum states localized on classical trajectories, the idea of decoherence, and so on.

Computational Methods of Molecular Physics Group

Jacek Kobus – head of the group, Jacek Karwowski, Grzegorz Pestka, Monika Stanke, Lech Cyrnek

The main research areas:

1. Finite difference Hartree-Fock method for diatomic molecules

The finite difference Hartree-Fock method has been developed and used to provide Hartree-Fock limit values of total energies, multipole moments, polarizabilities and hyperpolarizabilities for a wide range of diatomic molecules. The main application of the method is in providing benchmark values to facilitate the construction of universal sequences of even-tempered Gaussian basis sets and assessment of their quality.

Further development of the method aimed at including the correlation and relativistic effects and extending its applicability to linear three-atomic molecules is in progress.

2. Relativistic and correlation effects in few-electron systems

In non-relativistic quantum mechanics the most accurate variational approximations to the stationary state energies and wavefunctions of many-electron systems have been obtained using trial functions which explicitly depend on the internuclear distance. Relativistic generalizations of these approaches are developed and applied to the Dirac-Coulomb equation for two-electron systems. Further generalizations and improvements of the approach are in progress. The results of this research are expected to supply the most accurate energies and wavefunctions for few-electron systems.

3. Variational principle and the Dirac eigenvalue problem

An application of the Rayleigh-Ritz variational procedure to the case of the relativistic Dirac-Coulomb eigenvalue equation, although resulted in many successful implementations, is far from being trivial and there are still many questions to be addressed. The main source of the difficulty is the unboundedness from below of the Dirac Hamiltonian and the multi-component character of its wavefunction. The question how to control the behavior of the variational energy by using rather weakly constrained variational trial functions, motivated the formulation of a number of mini-max principles. The main research directions on this subject include studies on the performance of the mini-max methods, an analysis of unexpected and pathological variational solutions and also developing algorithms for securing the correct results.

4. Exactly and quasi-exactly solvable models

Many quantum-chemical methods have been derived in a more or less straightforward way from analytically solvable models such as the hydrogen-like atom or the harmonic oscillator. Analytically solvable models also supply invaluable opportunities for checking correctness and ranges of applicability of a variety of approximations. During the last decade several new quasi-analytically solvable models have been introduced to quantum chemistry and to atomic and molecular physics. Probably the most interesting and the best known is the model describing two interacting electrons confined in a harmonic oscillator potential. We are involved in studies of the properties of this and similar quasi-exactly solvable models.

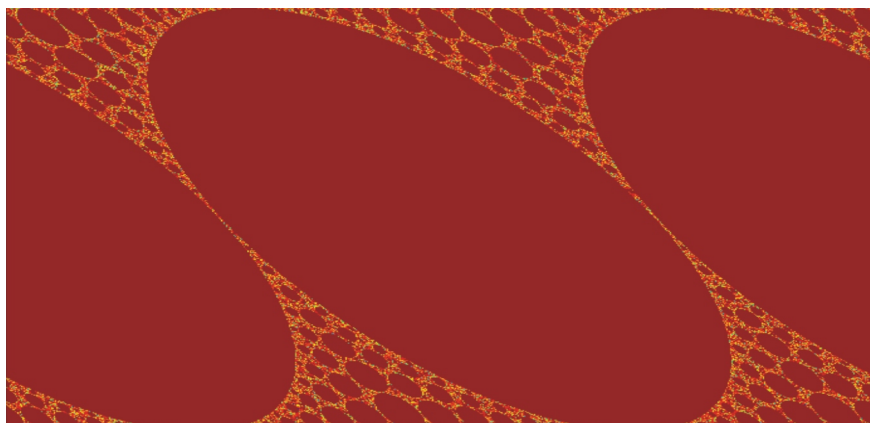
Dynamics of Open Systems Group

*Jan Iwaniszewski – head of the group, Stanisław Dembiński, Piotr Pełowski,
Piotr Matuszak, Piotr Weber, Aleksander Wozinski, Tomasz Zakrzewski*

All micro- or macroscopic physical systems interact with their surroundings and hence are open. The complete description of their dynamics requires the inclusion of some mechanisms of dissipation and fluctuations which result from this interaction. Contrary to common expectation that these perturbations would influence the dynamics only slightly, in many cases they lead to dramatic modifications of the systems properties. We are mostly interested in the dynamical aspects of this kind of problems, especially in the effects caused by time-dependent perturbations.

The main topics are:

- 1. Chaos in periodically perturbed systems:**
description of accelerating modes, tunnelling from chaotic to regular modes, properties of Floquet states, quantum fractals.
- 2. Thermal activation and tunnelling through fluctuating barriers:**
resonant activation, quantum-classical turnover, decoherence and localization.
- 3. Transport in classical and quantum systems subjected to periodical or random perturbations:**
stochastic ratchets, transport in coupled quantum-dots.
- 4. Statistical properties of lasers:**
transient states, polarization switching in VCSEL.
- 5. Signal processing:** applications of wavelet analysis to posturographic signals.

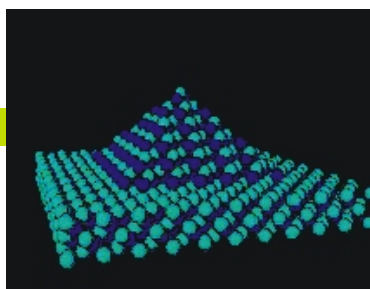


*Acceleration modes
of the gravitational bouncer*

Theory of Low-Dimensional Structures Group

Włodzimierz Jaskólski – head of the group, Mirosław Bylicki, Dorota Bielińska-Wąż,
Rafał Oszwałdowski, Artur Stachów, Michał Zieliński

A model of a self-assembled InAs quantum dot



The main research areas:

1. Microscopic theory of semiconductor quantum dots

Empirical tight-binding theory of strained nanoheterostructures is developed and applied to investigate electronic and optical properties of zero-dimensional semiconductor structures (systems of quantum dots). Resonance states and correlation effects in two-electron quantum dots are also investigated. The results of this research are important for modeling of quantum dot lasers, single electron transistors or quantum dot-based gates for qubit processing in future quantum computers.

2. Theory of surfaces and interfaces

Electronic structure as well as linear and nonlinear optical properties of semiconductor surfaces and interfaces are studied using density functional theory methods.

3. Confined many-electron systems

The influence of spatial confinement on properties of atoms and molecules is investigated. In particular, general relations between the form of the confining potential and the properties of the confined system are analyzed. The models of confinement studied include: the cylindrical parabolic confinement which may be used to describe the influence of an external uniform magnetic field, the spherical harmonic confinement which may emulate the external pressure, and the Debye (or Yukawa) screening potential, used to model the effects of plasma on the immersed atoms and molecules.

4. Carbon nanotubes

Electronic and transport properties of quantum dots and superlattices built of carbon nanotubes are investigated. Such systems lead to peculiar conductance features that can be exploited in all-carbon-based nanoelectronics.

5. Theory of atomic resonances

Highly-excited autoionizing states of few-electron atoms as well free as in presence of an external electromagnetic field or under the influence of a surrounding plasma are investigated. Energy levels and their widths are computed by using mainly the complex-coordinate techniques.

International collaboration:

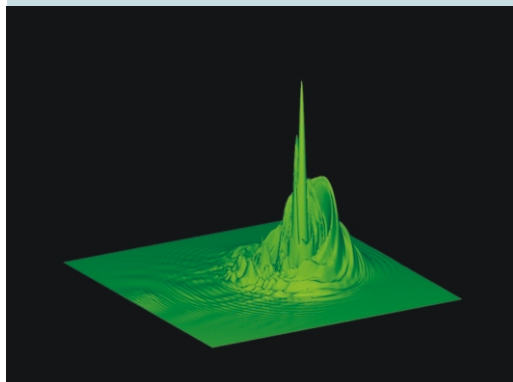
1. G.W. Bryant, National Institute of Standards and Technology, Gaithersburg, USA,
2. L. Chico, Universidad de Castilla-La Mancha, Toledo, Spain,
3. J. Planelles, Universidad Jaume I, Castellon, Spain,
4. C. A. Nicolaides, Technical University of Athens, Athens, Greece.

The inside of the strained InAs self-assembled quantum dot

Theoretical Spectroscopy Group

Lidia Smentek – head of the group, Andrzej Kędzioriski

The distribution of the probability of finding an electron during ultrastrong-field photoionization



The investigations are devoted to the theoretical description of spectroscopic properties of rare earth doped materials. The main emphasis of the research is directed to the understanding of the mechanisms that are responsible for the host sensitized luminescence of tissue selective lanthanide chelates. The research is inspired by the experimental evidence that the cages with the lanthanide ions are excellent probes for early detection of cancerous tissues in various organs of the human body. The uptake of the agent by various tissues strongly depends on the architecture of the chelates. A special role is assigned to the antenna that is responsible for the harvesting of the energy from the external beam, which in turn, is transferred to the lanthanide ion, excites it, and consequently leads to the luminescence that monitors the presence of cancerous cells. Unfortunately at this stage of knowledge it is not known and not even understood yet which physical mechanism is responsible for the energy transfer. Therefore there is a demand for a theoretical analysis that would provide information about the nature of the observed phenomena.

International collaboration:

D. Bornhop, Vanderbilt University, Nashville, TN, USA.

Quantum Optics Group

Andrzej Raczynski – head of the group, Jarosław Zaremba, Jacek Matulewski, Małgorzata Rzepecka

The group, for a long time informal, has been working already for about twenty years.

It is concerned with various aspects of light interaction with atomic systems. The main subjects of interest have been:

1. threshold effects in photoionization and photodetachment,
2. photoionization and photodetachment in strong laser fields: above threshold ionization (ATI),
3. photoionization and photodetachment in ultrastrong laser fields, adiabatic stabilization,
4. coherent population transfer and trapping in atomic systems including continuum states,
5. light propagation in the conditions of electromagnetically-induced transparency (EIT) and light storage,
6. charge transfer in DNA chains,
7. nonlinear optical properties of new organic materials.

The most important results were:

1. an examination of a nonexponential decay of the initial state population and of non-Lorentzian photoelectron spectra in near-threshold photoionization,
2. modeling the ATI photoelectron spectra within the time-dependent Keldysh-Faisal-Reiss approach,
3. proving the possibility of a population transfer between uncoupled bound states through a continuum, with the continuum-continuum transitions taken into account,
4. an investigation of multiphoton processes in calcium and in atomic hydrogen,
5. numerical simulations of electron photodetachment in ultrastrong fields; a demonstration of an adiabatic stabilization in one spatial dimension and its weakening in two dimensions; showing the possibility of restoring the stabilization in the latter case by using a constant magnetic field,
6. modeling light propagation and storage in three- and four-level atomic systems in the lambda and double lambda configuration; developing the polariton description of the dynamics,
7. study of nonlinear optical properties of new organic materials (TTF derivative).

The group has cooperated with the universities in Bielefeld, Kaiserslautern, Angers and Maynooth.

Head: Dr hab. Franciszek Firszt, prof. UMK

Prof. dr hab. Stanisław Łęgowski (emeritus)
 Prof. dr hab. Hanna Męczyńska,
 Prof. dr hab. Franciszek Rozpłoch
 Dr hab. Hubert L. Oczkowski, prof. UMK
 Dr Alicja Chruścińska,
 Dr Sławomir Kulesza,
 Dr Jaromir Patyk
 Dr Krzysztof Przegiętka,
 Dr Janusz Szatkowski,
 Dr Paweł Szroeder,
 Dr Jerzy Wieczorek
 Dr Jacek Zakrzewski,

Agnieszka Marasek, M. Sc.
 Lidia Nowak, M. Sc.
 Waldemar Marciniak, M. Sc.
 Lech Polakiewicz, M. Sc.

Ph. D. Students:

Khalid Benzour, M. Sc.
 Adam Dąbkowski, M. Sc.
 Zbigniew Nowak, M. Sc.
 Michał Pawlak, M. Sc.
 Karol Strzałkowski, M. Sc.

Physics of Semiconductors Group

Franciszek Firszt – head of the group, Hanna Męczyńska, Stanisław Łęgowski, Jacek Zakrzewski, Agnieszka Marasek, Michał Pawlak, Karol Strzałkowski

The scientific activity concerns growth and characterization of wide-gap II-VI binary compounds and their ternary and quaternary solid solutions with Mg, Be and Mn as constituents. The bulk crystals are grown with the modified high pressure Bridgman method from the melt under argon overpressure of 10–13MPa. The following materials are obtained: ZnSe, ZnTe, CdSe, CdTe, ZnMnTe, ZnMnSe, ZnMgSe, CdMgSe, ZnBeSe, CdBeSe, ZnBeTe, ZnMgBeSe, ZnCdMgSe, ZnCdBeSe and ZnMnBeSe. These semiconducting compounds are of interest for their potential application in optoelectronics (green laser diodes, visible and UV photodetectors, Bragg reflectors) and spintronics.

Radiative and nonradiative recombination processes, photoelectric, photooptical and photothermal properties of these semiconductors are studied. Photoluminescence and luminescence excitation spectra are investigated in the temperature range from 30K to room temperature. The excitonic energy gap can be determined as a function of composition and temperature. Luminescence measurements combined with photoconductivity spectra and decay of photoconductivity provide information concerning localization of excited carriers due to compositional and structural disorder. Photoacoustic spectroscopy technique with piezoelectric and pyroelectric detection is used for investigation of photothermal properties and nonradiative recombination processes. In particular, the energy gap and thermal diffusivity of the investigated materials are determined.

The group cooperates with Institute of Physics, Polish Academy of Sciences, Warsaw (investigations of structural and magnetic properties and determination of lattice constant and composition), University in Białystok and Helsinki (positron annihilation and Hall measurements), University in Bochum - Germany (photoacoustic and photothermal investigations), Bydgoszcz University of Technology and Agriculture, Poznań Technical University, University in Metz and National Taiwan University of Science and Technology.



Radiospectroscopy and Carbon Physics Group

Franciszek Rozpłoch – head of the group, Sławomir Kulesza, Jaromir Patyk, Janusz Szatkowski, Paweł Szroeder, Lidia Nowak, Waldemar Marciniak, Khalid Benzhour, Adam Dąbkowski, Zbigniew Nowak

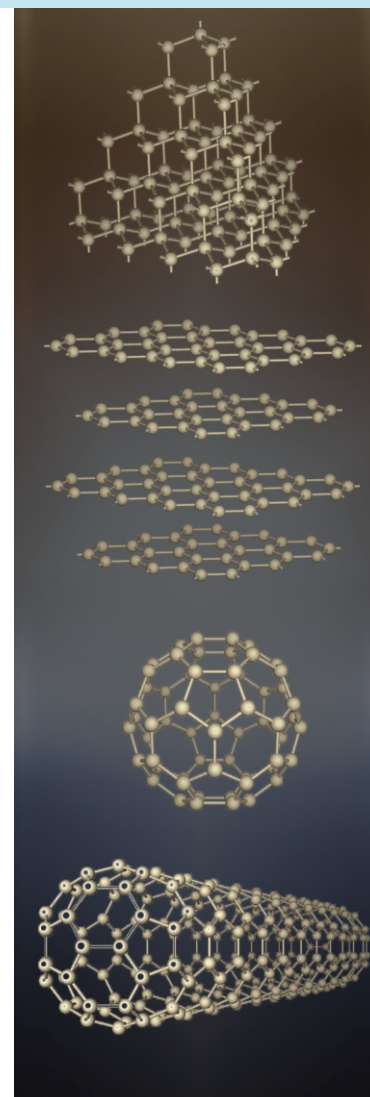
Carbon structures

In the early 1960s, Prof. Kazimierz Antonowicz initiated in Toruń the studies of carbon materials. Since then, the carbon research group has been investigating structural and electronic properties of different forms of carbon obtained by thermal decomposition of organic substances. The carbon-based structures of interest are: amorphous and glass-like carbons, carbon fibers, polycrystallite diamond films, pyrolytic carbons, graphite and its intercalates, fullerenes and nanotubes, which are related to pure 3D-allotropes of carbon — graphite and diamond.

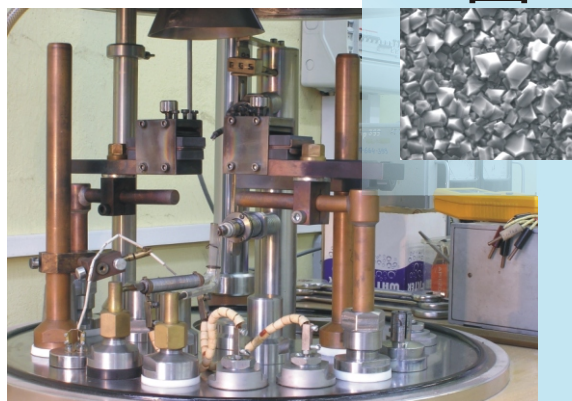
The main issues under consideration are:

1. **disordering effects in amorphous carbons,**
2. **defect- and disorder-induced localized electronic states** in the mobility gap of amorphous carbons,
3. **electronic states in the vicinity of the Fermi level in graphite derivatives** (carbon nanotubes, turbostratic graphite, graphite intercalates),
4. **high temperature electric transport mechanisms** in polycrystallite diamond and nanotubes,
5. **electric properties of fullerene's cations.**

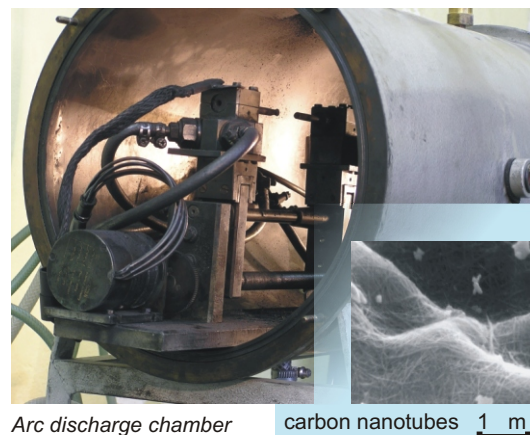
The group has developed arrangements for HF CVD and for the arc discharge synthesis. The manufactured materials are investigated by several experimental techniques: SEM, TEM, ED, XRD, EPR, Raman and IR spectroscopy. Measurements of surface electrical conductivity in a high temperature range are also carried out.



Arrangement for CVD synthesis



diamond 2 μ m



Arc discharge chamber

carbon nanotubes 1 μ m

Luminescence Dating Group

*Hubert L. Oczkowski – head of the group, Alicja Chruścińska,
Krzysztof Przegiętka, Lech Polakiewicz*

The dating laboratory of the Institute of Physics, at present called Luminescence Dating Group was established in 1988 as a part of the Interdisciplinary Group for Methods of Dating at Nicolaus Copernicus University. This interdisciplinary group consists of cooperating laboratories designed to deal with different subjects. The Luminescence Dating Group deals with the luminescence and dosimetry problems basic for the luminescence dating of geological and archaeological objects.

The staff of the group has carried on the research in the field of stimulated luminescence for thirty years. The early works concerned ZnSe. Recently, apart from the research of minerals related to dating problems, the group takes part in the investigation of scintillating materials.

The purposeful equipment of laboratory consists of high and low temperature thermo-luminescence (TL) arrangements. For the basic investigations of TL, the laboratory can carry out the Gobrecht-Hoffman analysis, which allows to study trap parameters. The multiplex spectroscopy arrangement records the TL spectra. TL/OSL reader (Riso TL/OSL DA-12) is used for dating. The dose rate survey is carried out using the multichannel gamma spectrometer (MCA100–Canberra).

A particular importance is attached to the scientific cooperation with the Department of Radioisotopes at the Institute of Physics of Silesian University of Technology and with the Dating Laboratory of the University of Helsinki.

The research activities of the Luminescence Dating Group aim at development of modern methods of absolute dating, especially for quaternary geochronology purposes.

The principal work areas are:

- 1. dating of geological and archaeological objects,**
- 2. fundamental research of the stimulated luminescence phenomenon,**
performed by the solid state physics methods,
- 3. joint research and cooperation aimed at laboratory problems**
that are specific for luminescence dating procedures.

Current interest of the group is determined by one of the main problems in luminescence dating for many years — the lack of an objective method enabling to prove the proper resetting of the sediment luminescence signal before the deposition. The “reset problem” provokes investigation of bleaching mechanisms and carrier transfer in minerals. The detailed knowledge of these processes could allow to introduce the selective procedures, which lead to the determining of the luminescence level before the sediment deposition.

In the field of dating, recent results obtained within the close cooperation with our colleagues from the Institute of Geography, helped to establish the evolution of the geomorphologic environment in the case of the early-mediaeval settlement site in Kałdus (Toruń’s vicinity). These investigations opened closer cooperation of the Luminescence Dating Group with archaeologists.



Gamma spectrometer

Department of Optoelectronics

Head: Prof. dr hab. Andrzej J. Wojtowicz

Dr hab. Czesław Koepke, prof. UMK
 Dr Winicjusz Drozdowski
 Dr Dariusz Wiśniewski
 Dr Krzysztof Wiśniewski
 Dr Bernard Ziętek
 Marcin Ptaszyk, M. Sc. technical staff

Ph. D. students:

Dawid Piątkowski, M. Sc.
 Łukasz Sikorski, M. Sc.
 Sebastian Janus, M. Sc.

The scientific team of the Department is involved in research in solid state physics, solid state spectroscopy and luminescence. The specific projects are concerned mostly with the optical properties of various solid state materials (crystals, glasses, ceramics) activated by rare-earth (RE) and transition metal (TM) ions that could potentially be used as materials for detectors of ionizing radiation (scintillators), lighting and display phosphors, and laser materials.

The Department is also responsible for undergraduate and graduate programs in optoelectronics and laser physics leading to M. Sc. and Ph. D. degrees. The optoelectronics course for students is devoted to the past, present and the future of some key areas of optics, and, in addition to the theoretical approach, covers many areas of applications, ranging from industry to communications.

The Department is composed of two research groups:

Laser Materials Group

Czesław Koepke – head of the group, Krzysztof Wiśniewski, Dawid Piątkowski, Łukasz Sikorski

The Group's field of activity is optical spectroscopy of the materials that could be potentially attractive from the laser point of view: crystals, glasses and polycrystallines (glass ceramics) activated by rare earth or transition metal (TM) ions. Apart from the standard spectroscopic data taken from the measurements of the absorption spectra, emission spectra, emission decays, luminescence excitation spectra and time resolved emission spectra, a special stress is put upon the excited state absorption (ESA) and gain measurements because they are of critical importance in determining whether a given material is a good candidate to be a laser gain medium. But even when there is no gain in the medium the ESA measurements still provide very useful and important data on the higher excited states. The ESA characteristics involve in general the ESA spectra or gain (wherever the net gain is possible) and the ESA decays. The Group focuses its attention mostly on trivalent RE ions (Pr^{3+} , Nd^{3+} , Er^{3+} , Ho^{3+} , etc.), but also on TM ions of different valency (e.g. chromium ions from Cr^{3+} up to Cr^{6+}) embedded in various prototype matrices. The most desirable goal is selection of novel tunable laser material working in the visible or UV. The observed phenomena are interpreted by means of the effects crucial for the laser efficiency: the ion-ion energy transfer, various radiationless transitions mechanisms, upconversion, influence of the defect states, trapped excitons, energy transfer upconversion etc.

The Group stays in informal collaboration with several laboratories at: the University of Leeds, Strathclyde University, Glasgow, Institute of Electronic Materials Technology ITME, Warsaw, Polish Academy of Sciences, Warsaw University of Technology and Gdańsk University.

The research is performed basing so far on grants from the Polish Committee for Scientific Research (KBN) and local Nicolaus Copernicus University grants.

Scintillator and Phosphor Materials Group

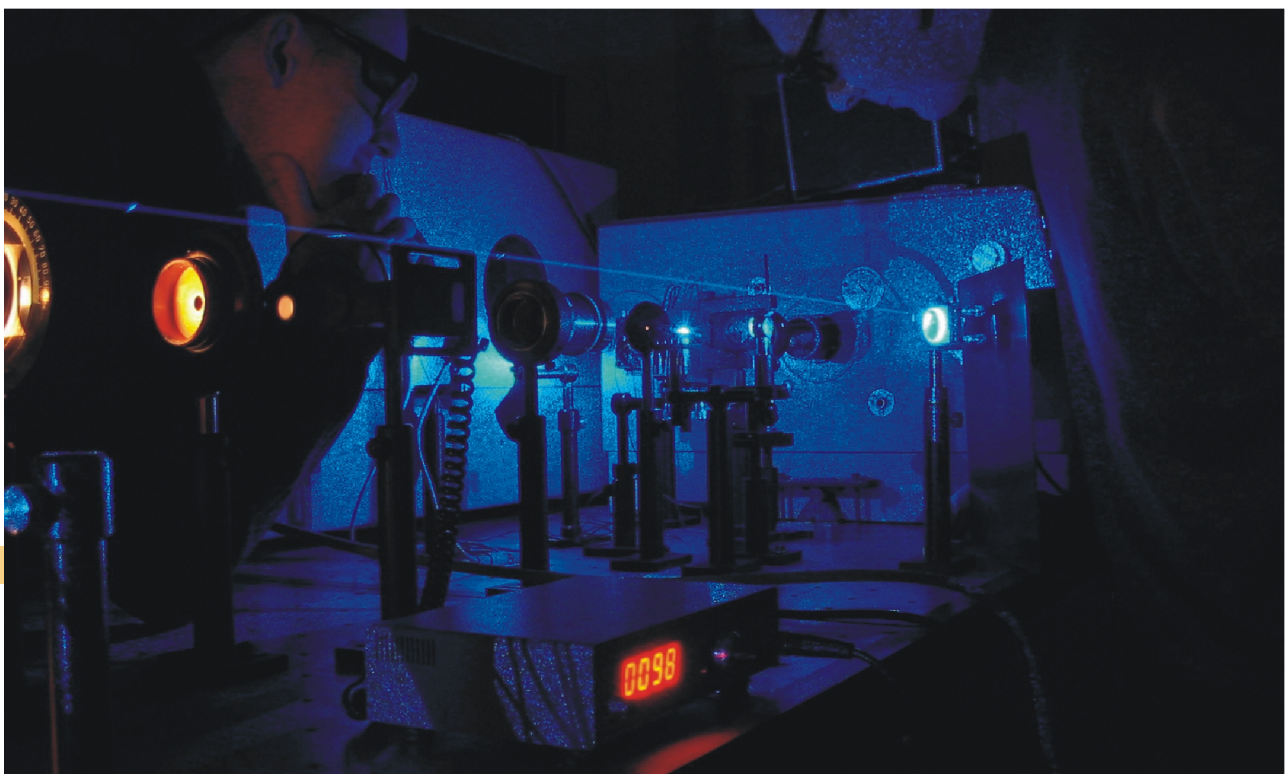
*Andrzej J. Wojtowicz – head of the group, Winicjusz Drozdowski,
Dariusz Wiśniewski, Sebastian Janus*

The main focus of the Group is on light production mechanisms in potential scintillator and phosphor materials, including recombination processes at structured impurities in wide bandgap optical materials. The electronic structure of systems comprising the activating ion and the solid state host material, and processes such as energy conversion and transfer mechanisms, luminescence and energy losses and radiation induced defects are the most important characteristics of material systems that the Group targets to study and describe. The ultimate goal the Group aims to achieve is to find a luminescent material that could be employed in practical devices extending the available wavelength range to UV and VUV. A carefully selected combination of a wide bandgap material and an appropriate dopant must be found that would support a fast and efficient radiative recombination using a full energy of the recombining electron-hole pair with no loss to lattice relaxation.

Some recent topics of interest include:

- 1. Radiative recombination and scintillation mechanism**
in new scintillator materials (LuAP, LuYAP, LSO, LYSO), garnets (YAG)
and alkaline earth fluorides (BaF_2 , CaF_2) activated with Ce and Pr,
- 2. Radiation damage centers** in perovskites, garnets and fluorides,
- 3. UV and VUV spectroscopy**
of perovskites, garnets and alkaline earth fluorides activated with RE ions,
- 4. Energy transfer and energy loss mechanisms**
in scintillator and phosphor materials activated with RE ions.

The Group collaborates with a number of European laboratories (Brussels, Hamburg, Delft, Geneva, Prague) and commercial companies (Photonic Materials Ltd, CTI Molecular Imaging Inc). The Group is involved in activities of the Crystal Clear Collaboration sponsored by CERN and European Community. Since 1997 it has been actively participating in research programs at Hasylab (VUV spectroscopy) in Hamburg, Germany. The members of the Group maintain also close links with other Polish laboratories in Warsaw (Institute of Electronic Materials Technology ITME, Polish Academy of Sciences, Warsaw University of Technology), Wrocław (Polish Academy of Sciences, University of Wrocław), and Szczecin (University of Szczecin) and are supported by grants from the Polish Committee for Scientific Research (KBN), commercial companies (PML, CTI MI), and European Community.



Department of Technical and Applied Physics

Head: Dr hab. eng. Marek Zieliński, prof. UMK

Prof. dr hab. eng. Krzysztof Gałkowski
 Dr hab. Wacław Bała, prof. UMK
 Dr hab. Jacek J. Fisz, prof. UMK
 Dr hab. eng. Lech Grzesiak, prof. UMK
 Dr Beata Derkowska
 Dr eng. Wiesław Hanus
 Dr eng. Kazimierz Karwowski
 Dr Zbigniew Łukasiak
 Dr Przemysław Płociennik
 Dr Zygmunt Turło
 Dr Anna Zawadzka
 Krzysztof Bartkiewicz, M. Sc.
 Piotr Borowski, M. Sc.
 Marcin Gahbler, M. Sc.
 Maciej Gurski, M. Sc.
 Eng. Andrzej Korcała, M. Sc.
 Anna Rożnowska, M. Sc.
 Eng. Andrzej Wawrzak, M. Sc.

Ph. D. students:

Artur Bratkowski, M. Sc.
 Łukasz Borszewski, M. Sc.
 Dariusz Chaberski, M. Sc.
 Paweł Dalasiński, M. Sc.
 Marcin Dębski, M. Sc.
 Krzysztof Domański, M. Sc.
 Robert Frankowski, M. Sc.
 Sławomir Grzelak, M. Sc.
 Izabela Kołupajło, M. Sc.
 Marcin Kowalski, M. Sc.
 Sławomir Mandra, M. Sc.
 Mateusz Rębarz, M. Sc.
 Michał Wojdyła, M. Sc.
 Leszek Wydźgowski, M. Sc.

Measurement and Control Systems Group

Marek Zieliński – head of the group, Krzysztof Gałkowski, Lech Grzesiak, Kazimierz Karwowski, Andrzej Wawrzak, Maciej Gurski, Dariusz Chaberski, Robert Frankowski, Marcin Gahbler, Sławomir Grzelak, Marcin Kowalski, Sławomir Mandra, Leszek Wydźgowski

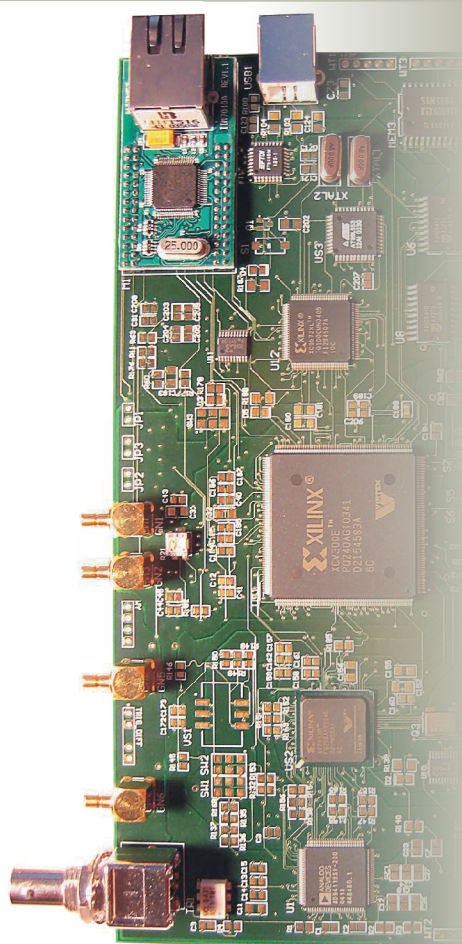
The main fields of interest of the group are: measuring systems, virtual instruments, digital signal processing, drive control systems and motion processors.

The investigations include: design methods, optimization of the measuring parameters, optimization of control systems and construction of devices.

In the field of measuring systems the group activity is focused on: precision time counters, time to digital converters, the Peripheral Computer Interconnect interface cards for the precision time-interval measurements, multichannel scalars, ultrasonics flowmeters and energy meters. As regards the drive control systems the subjects of interest are: microstepping step-motor controllers implemented in the Field Programmable Gate Array and Configurable System on a Chip devices, the computer numerical control multi-axis systems and synchronous motor systems for machine tools, manipulators and robots.

In particular the group is interested in the measuring systems implemented in unique programmable devices, e.g. reconfigurable time-interval measuring systems implemented in the structures of programmable devices. The group also works on application of such instruments to atomic physics experiments.

The group collaborates with the Research and Development centers of APATOR S. A. and OBRUSN Toruń.



Reconfigurable time-interval measuring system

Photonics and Optical Biospectroscopy Group

Jacek J. Fisz – head of the group, Anna Rożnowska, Marcin Dębski, Izabela Kołupajło

The main fields of interest of the group cover:

1. spectroscopy of the charge transfer molecular systems which may have a potential application in technology of organic photovoltaics,
2. spectroscopy of the systems undergoing excited-state process (CT, TICT, PT) in solutions and organized molecular media,
3. fluorescence studies of the structure and dynamics of polymers, Langmuir-Blodgett (LB) films and the models of biological membranes.

The group activity is focused on development of

1. numerical methods for global analysis of time-resolved experiments (gradient methods, genetic algorithms),
2. theoretical and experimental methods for variable-angle fluorescence depolarization studies of polymers, LB films and models of biological membranes,
3. theoretical and experimental methods in studies of thin molecular layers by means of the evanescent-wave-excitation fluorescence spectroscopy.

The group collaborates with several research centers in Poland and with several groups from abroad, including Lund, Berlin, Paris, Manchester, Trondheim.

Physical Foundation of Microelectronics Group

Wacław Bała – head of the group, Beata Derkowska, Wiesław Hanus, Zbigniew Łukasiak, Przemysław Płóciennik, Zygmunt Turło, Anna Zawadzka, Krzysztof Bartkiewicz, Piotr Borowski, Łukasz Borszewski, Artur Bratkowski, Paweł Dalasiński, Krzysztof Domański, Andrzej Korcala, Mateusz Rębarz, Michał Wojdyła

The main field of interest of the group is the electrical and optical properties of low-dimensional organic and inorganic semiconductor structures. Specifically, the research of the group is focused on thin epilayers of II–VI compounds, including ZnSe, ZnTe, ZnS, ZnSSe, ZnCdSe, ZnMgSe etc., and on the related quantum structures. The group prepares thin porous silicon layers, thin films of polymers (PPV, PCV), molecular organic crystals (PTCDA, Alq3, CuPc, ZnPc etc.).

Thin layers and multilayer structures of II–VI compounds and organic compounds are prepared by molecular beam epitaxy (home made system), pulse laser deposition, thermal evaporation and hot wall epitaxy methods. A wide range of optical, electrical and structural characterising techniques such as photo- and electroluminescence, time resolved spectroscopy, photoconductivity, optical absorption and photoabsorption, reflection and photoreflexion, photovoltage dependencies, Raman scattering, current-voltage characteristics, deep level transient spectroscopy, admittance spectroscopy as a function of temperature (10 – 350K) — are applied. Using these techniques, the energy band structures, interface states, impurity levels, exciton-phonon interactions, carrier concentration, deep levels, radiative and nonradiative recombination centers, and surface states, efficiency of electroluminescence are investigated.

Several space charge spectroscopy techniques [capacitance – voltage (C–V), admittance spectroscopy, thermally stimulated capacitance, Deep Level Transient Spectroscopy (DLTS), reverse DLTS] have been set up to investigate shallow and deep levels in II-VI, porous silicon and organic semiconductor structures. These techniques make it possible to determine the free carrier profiles (C–V) as well as the activation energy, the concentration and the capture cross section of deep levels located in the space charge region. The group investigates collective effects in low density plasma as results of laser radiation interaction with the matter and laser desorption/ionization effects on metal and semiconductor surfaces. Another field of interest is the electronic structure of thin films and surfaces.

The group maintains close collaboration with a number of research centers in Poland and abroad, including: Warsaw, Poznań, Bydgoszcz, Wrocław, Munich, Chemnitz, Hagen, Angers, Reims and Lille.

Department of Biophysics and Medical Physics

Head: Prof. dr hab. Aleksander Balter

Prof. dr hab. Andrzej A. Kowalczyk
 Dr hab. Wiesław Nowak, prof. UMK
 Dr hab. Piotr Targowski, prof. UMK
 Dr Danuta Jeziorek
 Dr Maciej Wojtkowski
 Dr Robert Zawadzki
 Waldemar Krychowiak, M. Sc.
 Stefan Meyer, M. Sc.
 Bogdan J. Szymański

The department members use both experimental (optics and optical spectroscopy) and theoretical (quantum chemistry and molecular dynamics) methods to investigate the structure and dynamic of biologically relevant molecules and tissues.

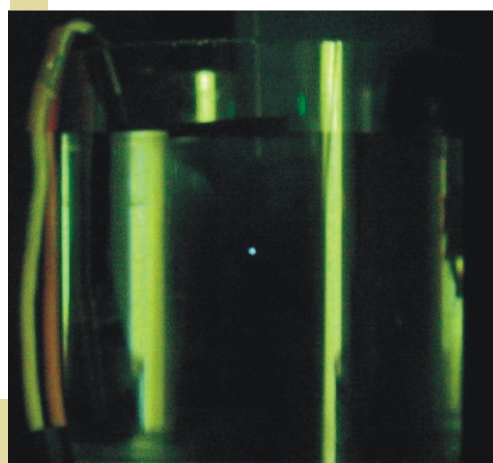
Experimental facilities include a time-correlated single-photon counting fluorometer with picosecond resolution, a double grating Raman spectrometer and a spectral-domain optical coherence tomograph with 6 micrometer resolution.

Computing resources include a cluster of PCs for parallel computations and several SGI graphical workstations.

In simulations we use NAMD, VMD, MOIL, InsightII, Discover, Gaussian, AutoDock and home made software.

Ph. D. students:

Tomasz Bajraszewski, M. Sc.
 Marta Cyganek, M. Sc.
 Bartosz Dobrzelecki, M. Sc.
 Iwona Gorczyńska, M. Sc.
 Karina Kubiak, M. Sc.
 Tomasz Łaska, M. Sc.
 Przemysław Miszta, M. Sc.
 Sławomir Orłowski, M. Sc.
 Łukasz Peplowski, M. Sc.
 Janusz Strzelecki, M. Sc.
 Anna Szkulmowska, M. Sc.
 Maciej Szkulmowski, M. Sc.
 Katarzyna Wiśniewska, M. Sc.



Single bubble sonoluminescence obtained in our laboratory

Aleksander Balter – head, Waldemar Krychowiak, Tomasz Łaska, Janusz Strzelecki, Katarzyna Wiśniewska

Research topics:

1. Luminescence and Raman spectroscopy of organic molecules in aqueous solutions

Luminescence and Raman spectroscopy methods are used to investigate the interactions between dissolved molecules and their environment. Currently our research is focused on interactions of xanthene dye molecules with metal nanoparticles.

2. Laser excited anti-Stokes fluorescence of organic dyes in solutions

Conditions and possible applications of laser excited anti-Stokes fluorescence of organic dye molecules e.g. optical cooling are investigated.

3. Molecular mechanisms of photodegradation

We study the influence of the UV and visible light irradiation on the properties of silver colloidal solutions in order to manipulate them optically. We also apply this technique to induce the photodegradation of tryptophan in order to elucidate the phototransformation pathways which may lead to the formation of the cataract in human eye lenses.

4. Generation of free radicals in foodstuffs

Mechanisms of free radical generation in foodstuffs by various factors including ultrasound, microwave, UV, Gamma, and X-ray irradiation are studied.

5. Mechanism of single bubble sonoluminescence

The mechanism of generation of picosecond light pulses by a single gas bubble trapped by an ultrasonic standing wave is investigated. Recently, we have demonstrated the possibility of controlling the light emission with an external electric field.

Collaboration

Prof. P.E. Marszałek, Center for Biologically Inspired Materials and MEMS, Duke University, Durham, NC, USA

Medical Physics Group

Andrzej A. Kowalczyk – head of the group, Piotr Targowski, Krzysztof Stefański (Collegium Medicum UMK), Maria Berndt-Schreiber (Faculty of Mathematics and Computer Science UMK), Maciej Wojtkowski, Robert Zawadzki, Tomasz Bajraszewski, Marta Cyganek, Iwona Gorczyńska, Anna Szkulmowska, Maciej Szkulmowski

Research topics:

1. Non-contact and non-invasive studies of ocular tissues

by the spectral optical coherence tomography:

- morphology of tissues 2-D and 3-D images, high resolution,
- functional studies, visualization of dynamics of morphological segments as well as pulsatile motion of blood vessels by tomographic movies, determination of blood flow velocity by phase measurements, determination of absorption in tissue as a function of axial depth,
- numerical methods for image improvement spectral shaping, Complex OCT, refraction correction, ray tracing,
- studies of physical limitations of optical coherence tomography,
- novel clinical applications — in cooperation with Collegium Medicum UMK.

2. Non-contact and non-invasive studies of art objects by optical coherence tomography:

- determination of the layered structure of the paintings and ceramics,
- studies of deformation caused by small changes of humidity and temperature.

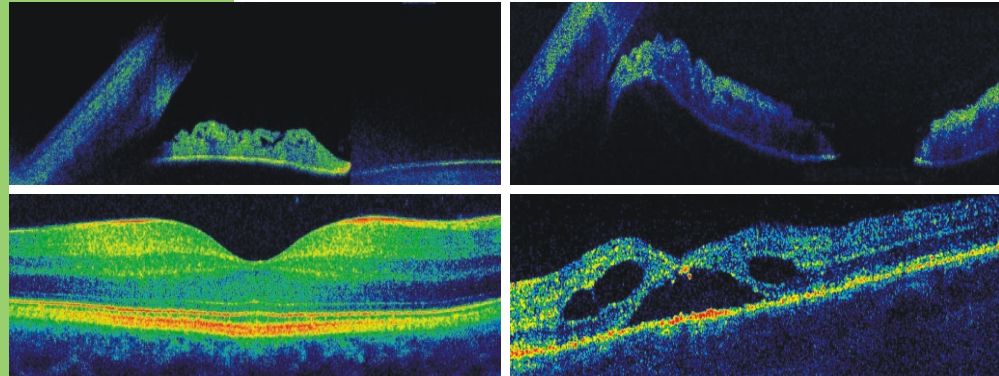
3. Advanced numerical analysis of images of fundus surface:

- search for relevant parameters obtained from image analysis of photographs of the fundus surface that might be correlated with various ocular pathologies,
- construction of an user friendly tool to administer large amount of data for future application in screening for glaucoma.



Optical coherence tomography examination

Optical tomograms of the anterior chamber (top) and the macula lutea (bottom) of the human eye in vivo. Left panels — normal subject, right panels — pathologies



Collaboration:

- Prof. A. F. Fercher, Institut für Medizinische Physik, Universität Wien, Austria,
- Prof. Ch. Hitzenberger, Centre of Biomedical Engineering and Physics, Medizinische Universität Wien, Austria,
- Prof. R. A. Leitgeb, Laboratoire d'Optique (LOB), Eidgenössisch Polytechnische Hochschule, Lausanne (EPFL), Switzerland,
- Prof. J. G. Fujimoto, Research Laboratory of Electronics, Massachusetts Institute of Technology, Cambridge, MA, USA,
- Prof. R. K. Wang, Cranfield Biomedical Centre Institute of BioScience and Technology, Cranfield University at Silsoe, Bedfordshire, UK,
- Dipl.-Ing. Dr. D. Stifter, Upper Austrian Research GmbH, Linz, Austria,
- Dr I. S. Ruddock, Department of Physics, University of Strathclyde, Glasgow, UK.

Department of the Theory of Many-Electron Systems

Head: Prof. dr hab. Karol Jankowski

Dr hab. Leszek Meissner, prof. UMK
Dr Ireneusz Grabowski

Ph. D. Students:
Jarosław Gryniakow, M. Sc.
Krzysztof Nowakowski, M. Sc.
Romuald Słupski, M. Sc.

The research activity of the division is mainly concerned with the development, reliability studies and pilot applications of new methods for theoretical studies of the electronic structure of atoms and molecules. Special attention is paid to the problem of description of electron-correlation effects by means of methods correctly describing the electronic states in the course of separation of the many-electron system into fragments (size extensive methods). So far, our activity has been concentrated on methods based on the nonrelativistic many-electron Schrödinger equation. However, recently we have started studies of the structure of the approximate exchange-correlation functionals employed in the dynamically developing Kohn-Sham density functional theory (DFT).

Our work on the problem of electron-correlation effects resulted in the development of several computational techniques:

1. A variation-perturbation method, based on the application of symmetry-adapted pair functions, especially designed for the treatment of larger atoms. This method allowed for the first time for systematic *ab initio* studies of electron correlation effects in larger atomic systems, including transition metals and rare-earth atoms. Results of the method have been broadly used as benchmarks in studies of the convergence of various basis sets to the complete basis set limits.
2. An intermediate Hamiltonian (IH) version of the valence-universal (VU) coupled-cluster (CC) method which removes many of the drawbacks of the standard effective Hamiltonian formulation. Main advantages of the new method are: state-specific character, many formal simplifications, and an effective way of solving the equations allowing one to efficiently deal with the intruder state problem.
3. An atomically oriented form of the valence-universal coupled-cluster approach based on one- and two-body radial cluster amplitudes (VU-CCSD/R method). Using this method it was possible to demonstrate that despite the common belief in the fatal effect of intruder states on the solvability of VU-CC equations, one can obtain solutions even for textbook examples of the intruder-state problem.
4. A valence-universal coupled-cluster method based on the concept of intermediate Hamiltonians formulated for handling atomic problems (IH VU-CCSD/R method). This method has been already applied to the Mg atom yielding very accurate energies for the ground state and some excited states.
5. A two-step approach describing the non-dynamical electron correlation within the multi-reference configuration interaction method and, next, accounting for the dynamical correlation effects when using a correction based on the single-reference CC analysis of the wave function. This scheme is effective both for ground and for excited states.
6. Simplified almost-linear versions of the CC approaches (AL-CC methods) based on a split-amplitude strategy of representing the cluster amplitudes. These methods are designed for applications to larger molecular systems.
7. A method of improving the performance of single-reference coupled cluster methods in applications to quasi-degenerate states by means of new types of *a posteriori* corrections.
8. A computational implementation of the *Ab Initio* DFT, which is universal and parameter free, for obtaining orbital-dependent exchange and correlation functionals based on many body perturbation theory (MBPT) or coupled-cluster methods.

Some other topics of current interest are:

1. Studies of the mathematical and physical content of the coupled-cluster equations and of the structure of the perturbation expansion for the energy. We have obtained for the first time the complete solutions to the CC equations. An analysis of their structure has led to a modification of the existing opinions concerning the pathological behavior of solutions to CC equations.
2. Reformulation of the genuine multi-reference coupled-cluster methods to make them simpler, more dependable, and numerically less demanding.
3. Formulation of hybrid methods which combine single- and multi- reference techniques for describing dynamic and nondynamic electron correlation effects.
4. Investigations of the impact of the choice of the reference functions on the efficiency of single- and multi-reference CC methods. A generalization of the Brueckner orbitals to the case of multi-reference model spaces has been proposed.
5. Development of new exchange-correlation functionals and potentials using the *Ab Initio* DFT , which allows one to directly exploit information from the wave function theory (WFT) based on the Schrödinger equation.
6. Studies of the structure and performance of the standard exchange-correlation functionals and potentials of the Kohn-Sham DFT by means of comparison with WFT results for large atoms.

Collaboration:

Department of Applied Mathematics, University of Waterloo, Canada;
 Quantum Physics Laboratory, Université de Paul Sabatier, Toulouse, France;
 Department of Chemistry, Princeton University, USA;
 Quantum Theory Project, University of Florida, Gainesville, USA;
 Departamento de Química Física, Universidad de Vigo, Vigo, Spain;
 Department of Chemical Physics, Comenius University, Bratislava, Slovakia.



The Education of Physics Laboratory

Head: Dr Józefina Turło

Dr Grzegorz Osiński
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 Elżbieta Dąbkowska, M. Sc.
 Andrzej Karbowski, M. Sc.
 Krzysztof Służewski, M. Sc.

The Education of Physics Laboratory (EPL) has been established in order to prepare physics students for elementary and secondary school teacher careers. The activity of the members of the group involves a faculty-based program of workshops, seminars and lectures as well as supervised teaching practices in schools. A range of courses devoted to various aspects of physics education is offered to students of physics and astronomy, postgraduate students as well as practising teachers (Postgraduate Courses on: Physics and Information Technology, Science, Environmental Studies, Information Technology in Science Education). The EPL staff is also active in co-operation at local, regional, national and international level.

Ultrasonic motion detector
constructed in EPL



The EPL activity includes:

1. **Participation in projects supervised and supported by the Polish Ministry of Education**, concerning mostly the IT based education and by the National Scientific Research Council on: „New Computer Aided Physics Experiments”. Two important solutions were obtained within these projects:
 - a. construction of continuous wave, ultrasonic motion detector for the measurements of the positions of two independently moving objects in the real time,
 - b. elaboration of hardware and software for computer aided ionizing radiation investigations (which we are also exporting).
2. **Preparation of educational TV programs** within the VIDEO-SCHOOL series, competitions for teachers and students, exhibitions of educational aids and demonstrations of physical experiments for teachers and students as well as writing expertises on textbooks, educational aids and multimedia resources.
3. **Organization of the national and international conferences:**
 - a. International Group on Physics Education (GIPEP) '91 on “Teaching about reference frames: from Copernicus to Einstein”,
 - b. “Computer aided experiments in physics education”, 1993–2003,
 - c. “Science and mathematics teaching for the information society”, 2000,
 - d. Polish Association of Science Teacher's annual meetings, 1994–2004.
4. **Collaboration with Polish science teachers** being the co-ordinator of international educational program: Science Across Europe and editing Polish Journal “Science Education”.
5. **Playing a role of contractor and co-ordinator of the TEMPUS program (1997–2001)** on: “Modernization of two-subject teacher education in physics and mathematics”. Within this program the collaboration between the EPL group and many european universities: Cambridge, London, Southampton, Leeds, Marseille, Amsterdam, Oldenburg, Kiel — has been established. As a result of the staff members and student activities several computer assisted learning techniques and multimedia capabilities have been up-dated and developed enabling applications in various fields of physics education.
6. **Being a Partner of EU SOCRATES projects:**

STEDE: “Science Teacher Education Development in Europe”, co-ordinator: University of Louvain, Belgium,

GRUNDTVIG: “Auto-formation et Auto-évaluation: Compétences et Connaissances pour des Etudes Scientifiques Supérieures” co-ordinator: Université de Provence, Marseille, France,

COMENIUS - EUCISE on: "European Union Co-operation on Integrated Science Education", co-ordinator: Institut für die Pädagogik der Naturwissenschaften, Kiel, Germany,

COMENIUS/EXPRESSTRAIN TEWISE 2.1 on: "Training Experimental Work in Science Education for teachers and teacher students", co-ordinator: Pedagogical Institute Carinthia-Department for Grammar School Education, Klagenfurt, Austria,

IP/AIDA Intensive Program on: “Attention-Interest-Desire-Action”, co-ordinator: Pädagogische Akademie des Bundes in Wien, Austria.

Head: Prof. dr hab. Włodzisław Duch

Dr hab. Jan Wasilewski, prof. UMK
 Dr hab. Jarosław Meller*
 Dr Krzysztof Grąbczewski
 Dr Norbert Jankowski
 Dr Antoine Naud
 Dr Sławomir Zelek
 Marek Grochowski, M. Sc.
 Halina Małek, M. Sc.

Ph. D. students:
 Łukasz Itert, M. Sc.
 Paweł Matykiewicz, M. Sc.
 Maciej Pilichowski, M. Sc.

Department of Informatics (DI, called until March 2002 the Department of Computer Methods) is an independent unit within the Faculty of Physics, Astronomy and Informatics, devoted to interdisciplinary research based on computational methods. DI is currently responsible for the undergraduate program in *computer physics*, leading to the M. Sc. degree, collaborates with the Institute of Physics on the informatics courses within the curriculum in technical physics, and with the Faculty of Mathematics and Informatics on the Computer Science curriculum.

Department of Informatics consists of two research groups:

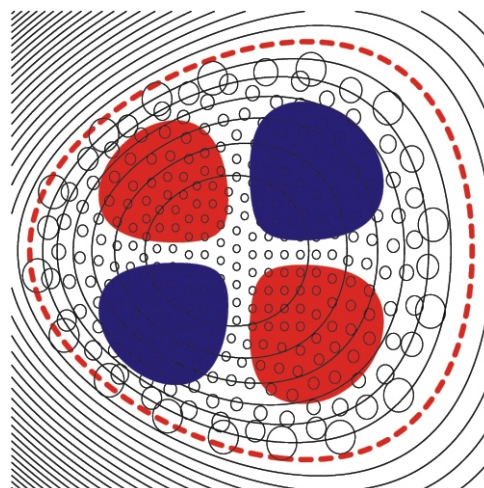
Computational Physics and Computational Biology Group

Jan Wasilewski – head of the group, Jarosław Meller, Sławomir Zelek

This group works on computational physics, theoretical molecular spectroscopy, quantum chemistry and computational biology. Among the goals of this research are development of methods for accurate description and analysis of properties of small polyatomic molecules, as well as state-of-the-art studies in theoretical molecular spectroscopy and molecular interactions. In particular, the group develops new mathematical methods for description and computer simulation of open-shell and multi-configurational molecular states, based on coupled cluster and density functional methods to solve the electron correlation problem. High quality calculations of potential energy surfaces for small polyatomic molecules and radicals are performed, with analysis of vibrational-rotational states and of the influence of the electron correlation effects on molecular constants.

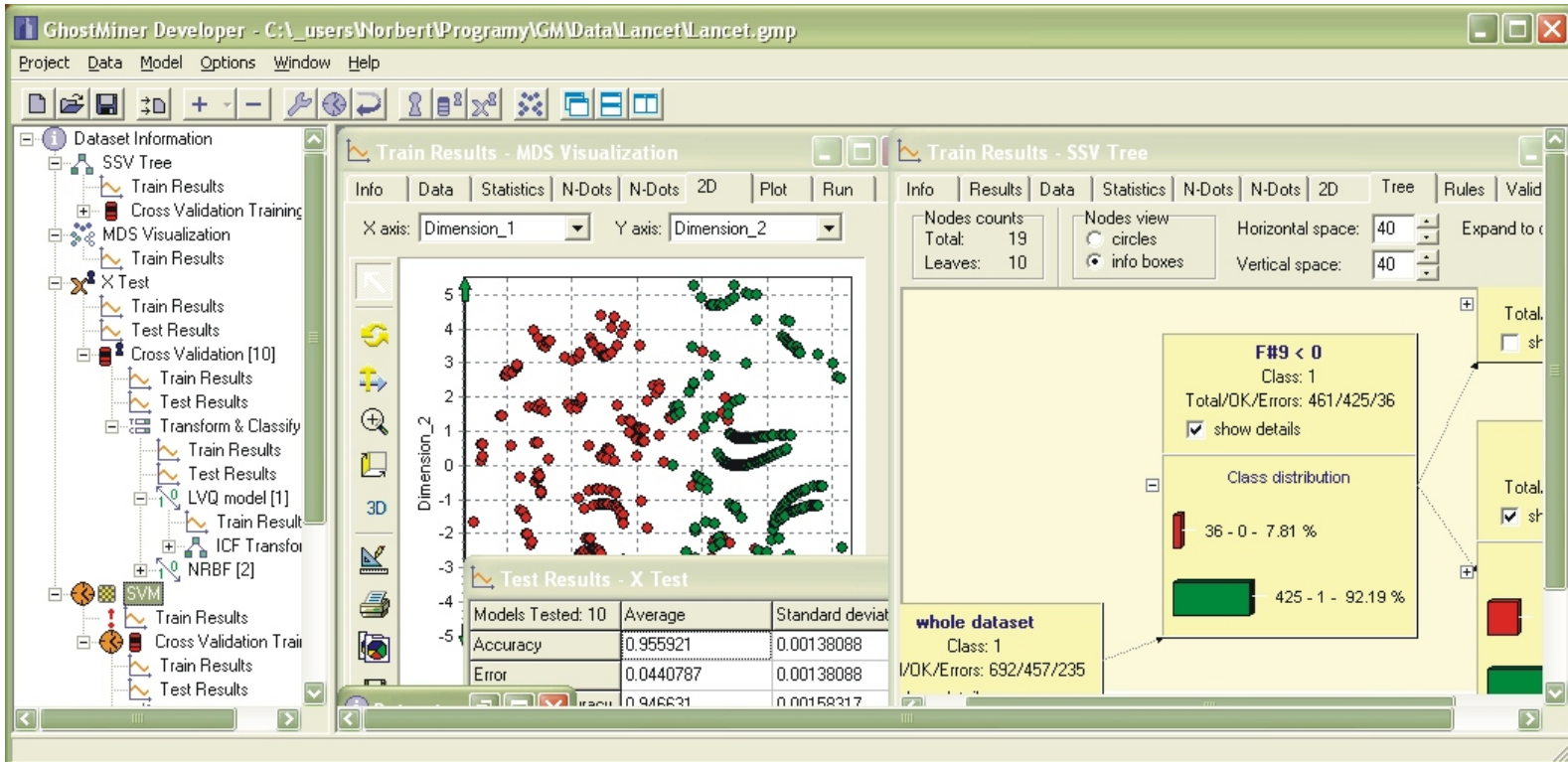
In computational biology (bioinformatics) the main research topics include: protein structure and function prediction, optimization of protein folding and threading potentials, gene identification and functional annotations algorithms, modeling of hormone and virus receptors and their interactions using molecular dynamics techniques.

Long-term cooperation includes research groups at the Ruhr University Bochum, Germany, Max Planck Institut für Astrophysik, Munich, Cincinnati Children's Medical Research Foundation, Cincinnati (Ohio), USA, Cornell University, Ithaca, USA, Hebrew University, Jerusalem, Israel, Kyoto University, Japan, and the Institute of Physics, Toruń.



Vibrational wavefunction for an AB₂ molecule, generated by DVR approach

*Also an Assoc. Prof. at the Department of Biomedical Informatics, Cincinnati Children's Medical Research Foundation, Cincinnati, USA.



GhostMiner data mining software developed in the Department of Informatics in cooperation with FQS Poland company

Computational Intelligence and Cognitive Science Group

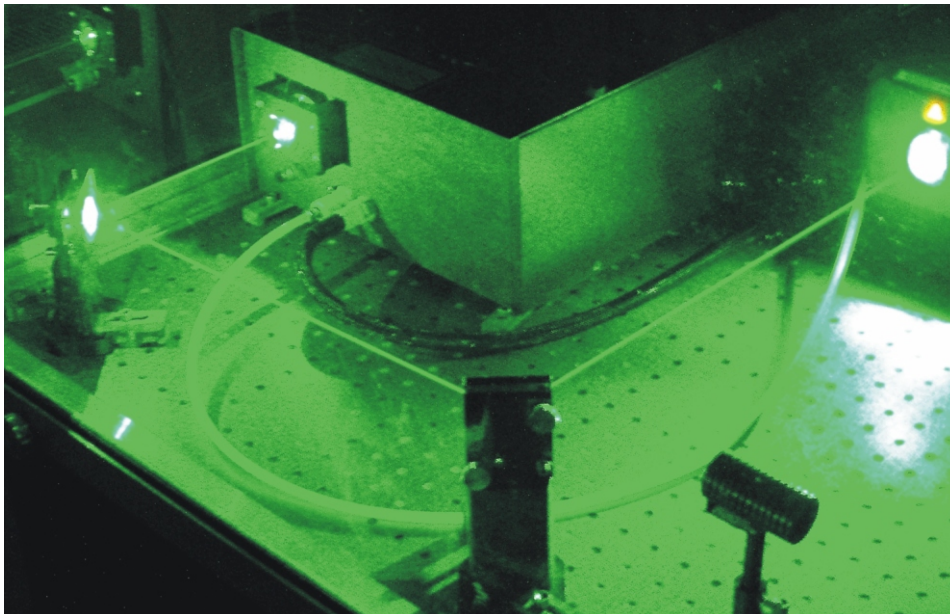
Włodzisław Duch – head of the group, Krzysztof Grąbczewski, Norbert Jankowski, Jarosław Meller, Antoine Naud, Marek Grochowski, Łukasz Itert, Paweł Matykiewicz, Maciej Pilichowski

This group works on development of theory and applications of **computational intelligence** (CI) methods, including neural networks, neurofuzzy systems, similarity-based methods, decision trees, visualization of multidimensional data, automatic knowledge acquisition and data mining. It has developed many interesting CI algorithms and has been involved in applications of such methods to analysis of scientific, technical, medical, and psychological data. Understanding of data, selection of information, and extraction of logical rules in various forms leading to automatic knowledge acquisition from examples, allows for construction of artificial intelligence expert systems for medical informatics, neuroinformatics, and bioinformatics applications. The goal here is to create new adaptive systems that can learn from data, create a theory that would encompass many such systems, implement theoretical results in software, and apply it to real-world problems.

The group has created a data mining software package *GhostMiner*, that is marketed by FQS Poland (Fujitsu group). Recently many projects in natural language processing are pursued, aimed at automatic creation of knowledge structures from text analysis, annotations of unstructured medical texts, development of question/answer systems and applications for word games.

Another area of research is applications of computational intelligence models in **cognitive science**, trying to understand how brains construct minds, how to use inspirations from such models to understand brain functions and dysfunctions. Recently this group has embarked upon a long-term international collaboration in development of a large scale **human brain simulator**. The group also takes part in several projects in **cognitive robotics** that will be pursued in the coming years as international collaborative efforts. These projects are aimed at construction of simulated talking heads and real android heads that should be able to communicate in a natural way with people, integrate graphics, behavioral control, speech recognition and processing, computer vision, various cognitive architectures, natural language processing and real time control. Variety of educational and other applications are envisaged. Some research in philosophy of mind, especially problems related to understanding consciousness and geometrical models of mind, is also being done by this group.

Long-term cooperation with research groups in Singapore, USA, and several European Union countries are maintained. This research is supported by grants from the Polish Committee for Scientific Research (KBN), commercial company (FQS), and grants from Singapore and USA.



National Laboratory for Atomic, Molecular and Optical Physics

National Laboratory FAMO* is a national-level research facility established to provide scientists with possibility of conducting the most-advanced experimental studies in atomic, molecular and optical physics in Poland. Some of the most important goals of the Laboratory are integration of the community of Polish specialists in the fields of FAMO and support of their participation in international scientific collaboration. Research activities of the Laboratory are carried out and supported by a multitude of scientists representing many Polish educational and research institutions. In return, many sophisticated scientific instruments, gathered in the Laboratory, unique in the scale of the Country have been made available to use by all researchers.

*FAMO is an acronym of *Atomic, Molecular and Optical Physics* in Polish.





Library

Head: Maria Jankowska, M. Sc.

Iwona Stęпка, M. Sc.
Ewa Reńska

Collections and activities

The collection consists of about 26000 volumes of books, mostly in physics, but also in mathematics (ca. 6000 vol.), chemistry, biology, astronomy, medical physics, microelectronics, automatic processes and computer metrology, to the extent dictated by the scientific interests of the faculty. In addition, the library collects scientific journals, the number of ongoing subscriptions being 90, i.e. 50 western titles, 8 Russian, and 32 Polish ones. On-line bibliographic reference data bases (e.g. INSPEC, PROLA) are also available.

Approximately 75% of the book collection is foreign, mostly in English and in Russian. One of the objectives is to acquire all Polish publications in physics and related areas, so as to keep the Polish collection as complete as possible.

Two catalogues are maintained: the alphabetic and the topical one. Since 1993, a computerized catalogue based on the ISIS system has also been constructed. Currently, the records cover about 95% of the library stock and are successively updated. Since 2000 all the new acquisitions have been included in the HORIZON basis (about 1800 records). Since 2002, the information on new acquisitions is available in the data base NUKAT.

There is a separate collection consisting of Ph. D. dissertations and M. Sc. theses (2925 items) authored by graduate students and faculty of the Institute of Physics. Since 1990, an ISIS-based computerized bibliography of publications by the faculty has been maintained. Presently, this data base contains 2240 records.

Experimental research interests, including ongoing activities and future plans, are:

1. Cold matter:

Atoms

- cold atoms in optical traps and lattices,
- cold atoms at surfaces,
- quantum degeneracy of bosons (Bose-Einstein Condensate) and fermions,
- cold collisions;

Atom optics,

Small ensembles of ions
in electromagnetic traps.

2. Quantum engineering:

fundamental problems,
quantum computing,
quantum control.

3. Biophotonics — applications of FAMO methodology and instrumentation in biology and medicine.



The library is rich in early volumes of the most important journals.

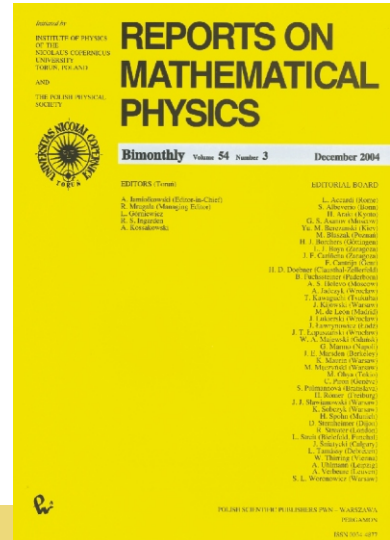
Physics Journals Edited in Toruń

Reports on Mathematical Physics

Bimonthly, published by Polish Scientific Publishers and Pergamon (Elsevier Science Ltd.)

Editors (Toruń): A. Jamiółkowski (Editor-in-Chief),
R. Mrugała, L. Górniewicz, R. S. Ingarden, A. Kossakowski

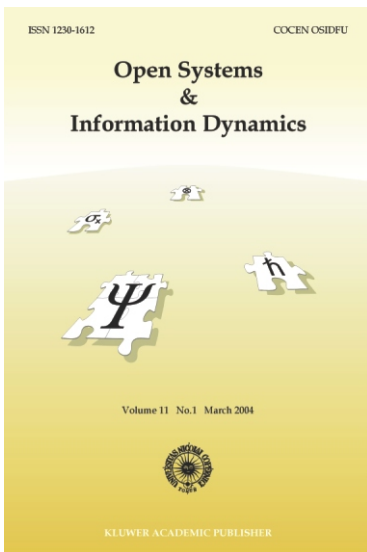
The journal was initiated in 1970 by the Institute of Physics of Nicolaus Copernicus University and by the Polish Physical Society to publish papers in theoretical physics which present a rigorous approach to problems of quantum and classical mechanics, dynamical systems, field theories, relativity and gravitation, statistical physics, and mathematical foundations of physical theories. Priority is given to papers with a direct connection with physics and papers using modern methods of functional analysis, group theory, differential geometry and topology, probability theory, algebra, etc.



Open Systems & Information Dynamics

Quarterly, published by Kluwer Academic Publishers

Editor-in-Chief: M. Ohya (Tokyo),
Co-Editors-in-Chief: L. Accardi (Rome), R. S. Ingarden (Toruń), A. Jamiółkowski (Toruń),
Managing Editor: P. Staszewski (Toruń), Leading Editors: J. Jurkowski (Toruń), M. Michalski (Toruń)



Aim and scope

The aim of the Journal is to promote interdisciplinary research in mathematics, physics, engineering and life sciences centered around the issues of broadly understood information processing, storage and transmission, in both quantum and classical settings. Our special interest lies in the information-theoretic approach to phenomena dealing with dynamics and thermodynamics, control, communication, filtering, memory and cooperative behavior, etc., in open complex systems.

The following topics are particularly welcome:

1. theory of quantum information, including quantum entanglement and measurement, quantum communication, computing and cryptography;
2. open systems and decoherence;
3. neural networks and genetic models;
4. information/entropy flow in complex dynamical systems;
5. other models of information processing.

The Journals are indexed/abstracted in:

COMPUMATH Citation Index; Current Contents/Engineering, Computing and Technology; Current Contents /Physical, Chemical and Earth Sciences; INSPEC Information Services; The ISI Alerting Services; MATH; Science Citation Index Expanded; Statistical Theory and Method Abstracts; Zentralblatt MATH.

Conferences ■

1. International Symposium on Mathematical Physics — organized annually in Toruń by the Department of Mathematical Physics (Chairman: A. Jamiołkowski). The 37th Symposium is planned for June 16–18, 2005,
2. International Workshop on Information Dynamics — organized biannually by the group associated with the journal *Open Systems and Information Dynamics* and with the International Society of Open Systems. Five Workshops (there were nine altogether) took place in the Institute of Physics UMK, (Chairman: P. Staszewski). Since 2003 the Workshop has been organized jointly with ISMP (see above),
3. Torunian Carbon Symposium — organized cyclically in Bachotek by the Group of Radiospectroscopy and Carbon Physics together with the Polish Carbon Society (Chairman: F. Rozpłoch). The seventh Symposium is planned for August 31 – September 3, 2005,
4. Nanostructures: Research, Technology and Applications — seminars organized cyclically in Bachotek by the Group of Physical Foundations of Microelectronics (Chairman: W. Bała). The eighth seminar is planned for May 18 – 21, 2005,
5. International Conference on Artificial Neural Networks ICANN2005 — the 15th Annual Conference of the European Neural Network Society is organized in Warsaw, September 11 – 14, 2005, by the Department of Informatics of Nicolaus Copernicus University and the Systems Research Institute of Polish Academy of Sciences, (Chairmen: W. Duch and J. Kacprzyk),
6. BioInformatics in Toruń BIT — a workshop organized annually by the Group of Theoretical Molecular Biophysics and the Department of Informatics (Chairmen: W. Nowak, W. Duch, J. Meller). The fifth BIT is planned for September, 15 – 16, 2005 as a satellite workshop of ICANN,
7. Symmetry, Spectroscopy, SCHUR — Brian G. Wybourne Memorial Conference – organized in Toruń by the Department of Quantum Physics; planned for June 12 – 14, 2005 (Chairman: R. C. King),
8. International Symposium of 50th Anniversary of the Expiry of Professor Jan Czochoński — Toruń, April 26, 2003 (H. Męczyńska and A. Zajączkowska),
9. ULTRA School on Ultrafast Processes in Photochemistry and Photobiology — a school organized within the ULTRA program financed by ESF; Toruń, August 25 – 30, 2003 (Chairman: J. J. Fisz),
10. The 36th Meeting of Polish Physicists — Toruń, September 17–20, 2001,
11. International Workshop Atomic Interactions in Laser Fields — Toruń, September 1 – 3, 1999 (Chairman: S. Chwirot) was one of a series of workshops which took place in Paris (1985), Duesseldorf (1987), Soesterberg (1989), London (1991) and Bad Honnef (1996),
12. Polish-Lituanian Workshop on the Semiconductor Physics and Technology — the eighth one took place in Toruń, June 28 – 29, 1999,
13. The Jabłoński Centennial Conference on Luminescence and Photophysics — Toruń, July 23 – 27, 1998 (Chairman: J. S. Kwiatkowski),
14. Spin-Orbit Coupling in Chemical Reactions — organized within the REHE program of EC (Chairman: J. Karwowski) Toruń, January 24 – 27, 1998,
15. PHARE–TEMPUS–TESSA Workshop on Computers in Education and Environmental Studies for science teachers was organized by the Physics Education Laboratory, August 21 – 25, 1995,
16. 23rd Conference of European Group for Atomic Spectroscopy EGAS Toruń, July 10 – 13, 1991, (Chairman: S. Łęgowski),
17. International Conference of Physics Education GIREP'91, *Teaching About Reference Frames: From Copernicus to Einstein*, Toruń, August 19 – 25, 1991, (Chairman: A. Jamiołkowski, Secretary: J. Turło).

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