Self-assessment report for the previous 4 years

Brief history and general description of the institute

Our institute was originally founded in 1950, as Physics Department of the Romanian Academy, branch of Cluj Napoca; 6 year later Institute of Atomic Physics (IFA) is founded in Bucharest and the institute becomes a subsidiary of IFA Bucharest.

The first benchmark in our development was in 1970 when the Cluj Section of IFA gets legal autonomy, under the name ***Institute for Stable Isotopes***, its main goals being R&D of heavy water technology. Soon however the research scope became broader and new directions of investigations developed at fast pace. For example separating and detecting stable isotopes, design and manufacturing of scientific equipment for isotope applications were topics growing in dimensions and importance.

As a consequence of this development, in 1977 the Institute for Stable Isotopes changes his name into ***Institute for Isotopic and Molecular Technology ITIM Cluj-Napoca***, having legal personality under the authority of State Committee for Nuclear Energy. The maximum of Institute development for this period was in 1989 when a total of 440 staff was involved both in research and in production of scientific instrumentation for important industrial customers like for example „Romag" heavy water production plant and Cernavoda nuclear power plant.

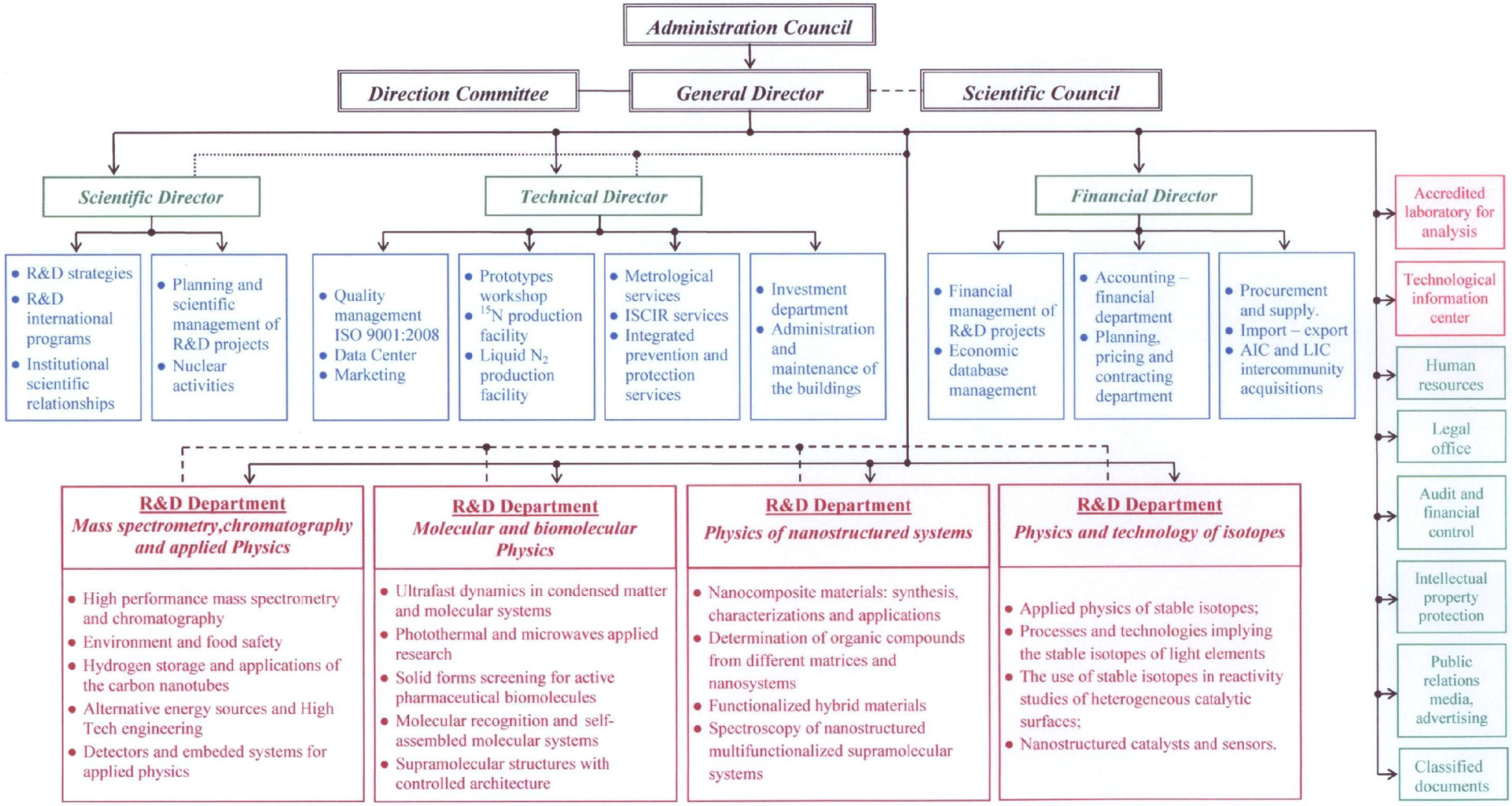
After 1990 our institute folows, durring a decade, the national decreasing trend of the research. It was a decay period with malefic effects, with consequences extending up to present days.

The second benchmark happens in 1999 when ITIM Cluj-Napoca is transformed into the ***National Institute for Research and Development of Isotopic and Molecular Technologies INCDTIM Cluj-Napoca*** (HG 408/1999). This moment marks the revival of the research and initiates the growth of institute.

Today INCDTIM is the only national institute for research and development in the north-western region of Romania. Having facilities at European standards, the institute offers a favorable environment for young people who aspire to a research career in physics areas like: mass spectrometry, chromatography and ion physics, physics of nano-structured systems, molecular and biomolecular physics and technology of stable isotopes.

Research is carried out in four departments (see 2.1. Administrative structure diagram of the institution) comprising 13 research teams, presented later in this report. The diagram also shows the structure and management levels and all related and administrative activities, to support research and technological development and innovation in the institute.

2.1. Administrative structure diagram of the institution



Hierarchical relationships : ⟶ direct subordination; - - - - collaboration; ····· subordination through delegation of duties.

2.1. General activity report of the institution

INCDTIM has established, in the framework of the national strategy on research, development and innovation for the period 2007 - 2013, the following main areas of R&D :

- Stable isotope separation and applications
- Production of isotope labeled compounds
- Multifunctional nano-structured materials (carbon nanotubes, functionalized metallic, polymeric, magnetic and composite nanoparticles, nanogels)
- Molecular and bio-molecular materials with controlled architecture and functionality (preparation, physic-chemical and structural characterization, practical applications: inclusion compounds, solid forms screening of active pharmaceutical ingredients)
- New multi-technique approaches for molecular systems characterization (combined solid-state NMR, X Ray diffraction, and molecular modeling; new photo-pyroelectric spectroscopy and calorimetric techniques)
- Organic mass spectrometry, chromatography, and ion physics
- Materials and technologies for hydrogen production and storage
- Applied physical systems (analytical equipment design and production, ion optics)

INCDTIM's institutional evolution in the 2007-2011 time range was generally positive but, however, with fluctuating growing rates depending on the negative impact of the fund cuts we had to face as an effect of the latest years recession. The growing process started in 2005 with the major aim of revitalizing research and innovation, and was therefore focused on the following strategic directions:

1. Quantitative accumulation of new logistics, combined with modernizing the research related assets – this means, rehabilitation of the laboratories, and, in many cases, the acquisition of new research equipment, of latest generation ;
2. Improve the Institute's human resource both, by attracting young research personnel, and increase their level of expertise, including through international mobility ;
3. Diversify our research directions, in the sense of adapting them to the European / international demands, but, however, by preserving at the same time the traditional areas where INCDTIM is recognized a leading actor in the Romanian research landscape ;
4. Increase the number and the importance of the applied research projects up to the point of reaching the zone of potential technological transfer, and determine a sizable effect in real economy. We have started the process by accessing EU funded projects, and attracting private research funds ;
5. Orient the research towards obtaining quantifiable results and increase its efficiency, for instance by reducing bureaucracy and also by implementing specific institutional and project management tools ;

6. Strengthen institutional collaboration with academic and research centers at both, national and international level: this has evolved from informal relationships, to complex cooperation within different bilateral or EU projects (FP6 and FP7) ;
7. Increase the Institute's visibility to the scientific community, but also to the society in general, which is important for disseminating the role of research in the modern world, and the utility of spending public money in this area ;

It is not possible to quantify the results of our research in an absolute way, without making a reference to an essential factor governing any economical sector – the financial situation over the last years. Within this context, we make a brief presentation of the economical figures with the most significant influences upon the Institute's proper functioning – the turnover, resulting primarily from research projects, the extra income resulting from economical activities, and the wage cost (Fig.1.).

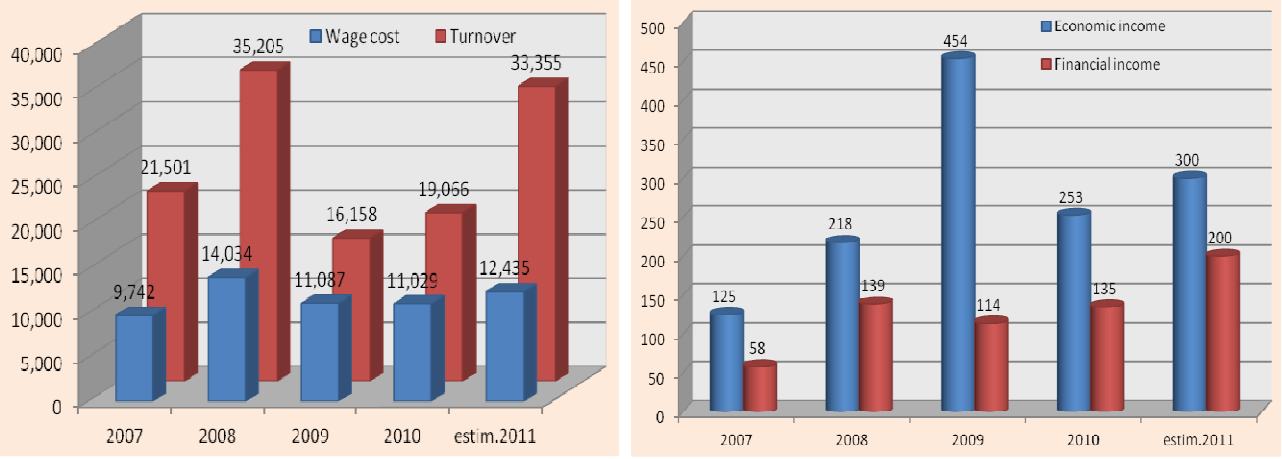
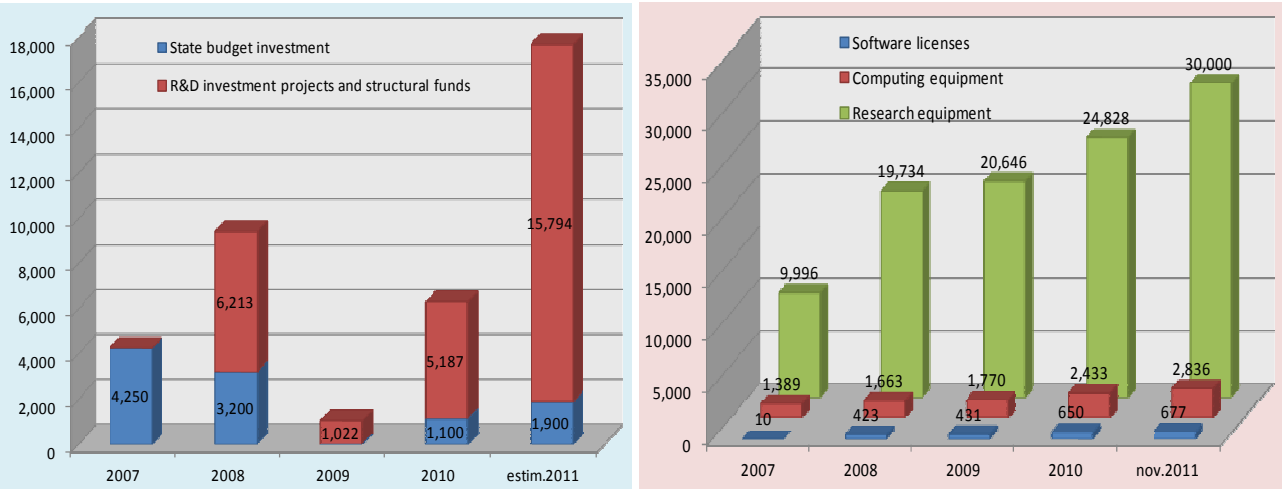


Fig.1. Economical and financial results [x 1000 lei], between 2007-2011.

A major component in the turnover is represented by the investment value. The investment funds have followed an increasing trend within the last four years, however, with large annual variations, both in amount, source, and destination. (Fig.2.).



a. b.

Fig.2. Annual evolution of investment funds (a) and accumulated value (b) [x 1000 lei].

From the above graphics it comes out very clearly a reduction in 2009 of all these parameters as an effect of the economic crisis, but also that this is followed by a constant increase up to the present. The major impact of the crisis was upon the investments from public funds. The fund cuts have been compensated by the financing with almost 21.5 million lei coming from several projects in the "Capacities" national program, and 3.3 million lei EU funds obtained from three European projects in the POS-CCE frame (structural funds).

Using public and own funds we have finished the rehabilitation of more than 90% of our research spaces, and also a new building that hosts the entire administration was built. The logistics has also been renewed: more than 70 % of the research equipment is newer than10 years, whereas 45 out of the 54 de equipments with value greater than 15.000 € have been acquired in the last 4 years. It is to be mentioned that all of these equipments are amongst the most performing on the market, while some of them are unique at regional or even national level. The modernized research infrastructure has now a very important impact upon our capability to perform research at the highest possible level, and attract in this way more national and European research projects.

The positive evolution of the research infrastructure (laboratories and equipment), has created the condition for profound qualitative changes also in our research activity. In this way, the necessity for comparable evolutions in the quality of the human resource has also occurred, in the sense of increasing the research potential by considering two important pillars: increase the number of the researchers, and enhancing their level of expertise.

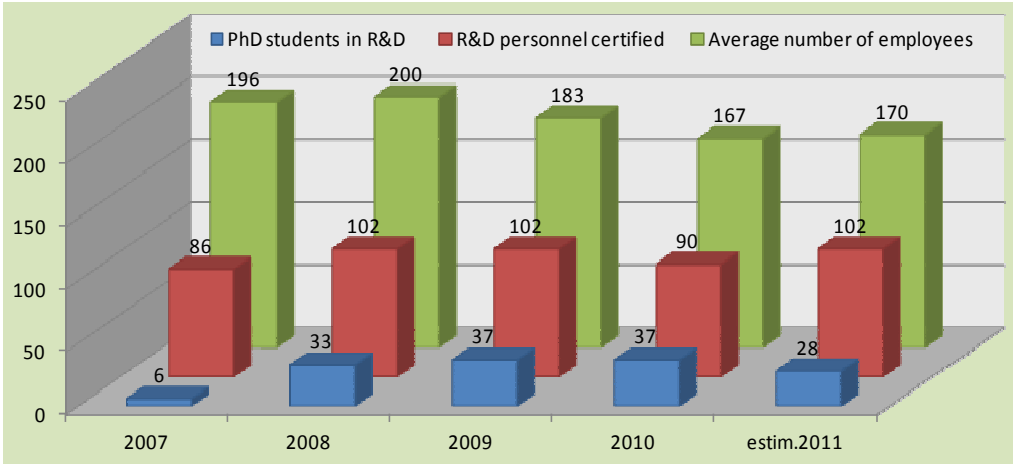


Fig.3. Annual evolution of R&D personnel – number and distribution, between 2007 – 2011.

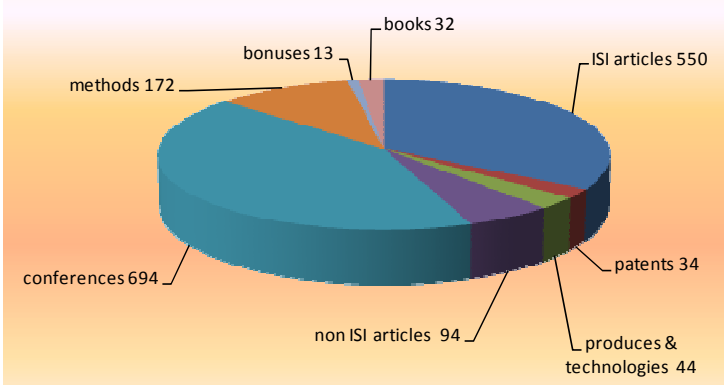
By attracting a larger number of young researchers to work at the Institute, the average age of the research personnel also dropped significantly in the last years: this was 57 years in 2007 compared to 43 years as it stands now. To achieve a high degree of specialization for the young researchers, two important measures have been considered: return of researchers specialized in important research centers abroad, and hiring graduate students, who have then followed intensive PhD stages funded by the Institute, most of them including also short training stages abroad. It is to be mentioned that in the present there are 71 researchers with the PhD title, and 33 PhD students,

out of 127 graduated persons working in the institute – directly in R&D, or as administration or support personnel.

The scientific level of the researchers from INCDTIM is certified by the large number of projects proposed to all types of competitions organized during last years at national and international level and by the high success rate. Practically speaking we won projects to all types of projects: PNI, PNII, structural projects, international bilateral, FP6 and FP7. As an example, at the last PNII IDEAS competition, from 28 proposals, after an international evaluation, 13 were financed. The 46.4% success rate was never reached before and represents clear-cut proof of the high level of competence and competitiveness.

If the number of the projects won at various competitions is enough to financially support the research activity of the institute, the efficiency of the scientific activity needs some quantified results. An efficient research produces results over the whole scientific range, from „*ab initio*" studies, up to patents and/or end products technologically transferable. The total amount of our results, obtained in the period 2007-2011 is displayed in the following diagram (Fig.4.).

Fig.4. Amount and distribution of R&D results, between 2007-2011.



The most important results quantifiable in our field of research are the papers published in ISI journals. The scientific impact of a paper is also determined by the number of citations and by the period of time in which the results keep the attention of the scientific community (Fig.5.)

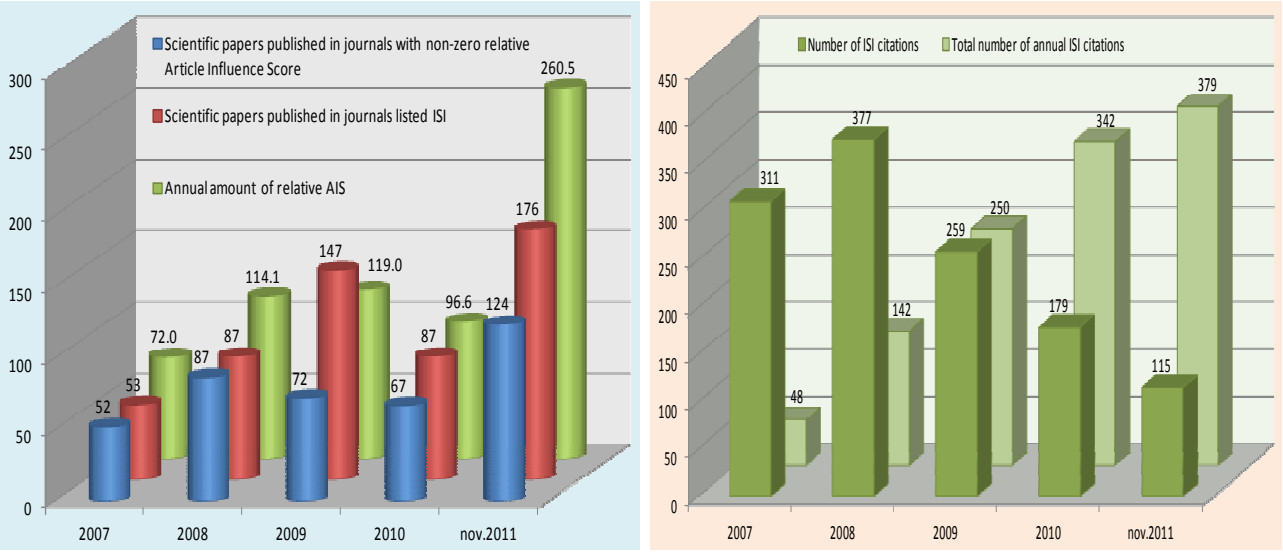


Fig.5. Evolution of scientific papers, published in ISI rated journals, between 2007-2011.

The presentation of valuable papers at international conferences brings at least two types of benefits – the information on the national/international level in the field and the opening of opportunities for joint bilateral or European collaborations. In the case of applied research, especially when the final product is technologically transferable, an important result is the patent, absolutely necessary to protect the author copyrights. However, patenting in developed countries is rather difficult, often prohibitive especially due to the huge taxes.

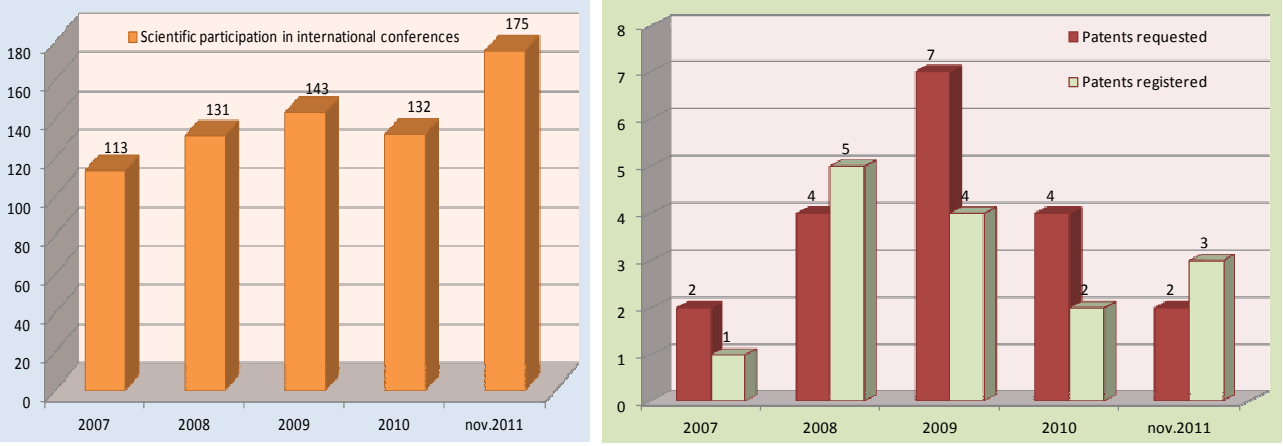


Fig.6. The participation in international conferences and the patent claim, between 2007-2011.

The economic results of the Institute come primarily from the contribution of the ^{15}N separation facility, which is unique in Europe, and also from the physico-chemical analyses performed for various customers by the ISO 17025:2005 certified Laboratory.

Prototyping workshop is well equiped, including with a CNC milling machine, has the cappability to produce complex mechanical components necessary for the High Tech prototipes required in some of the research projects: the most important in this sense are the international cooperation projects with ***CERN*** Geneve and ***Thales Optronics*** France.

The Institute's Data Center has a total processing cappacity of 5760 Gflops – over 600 cores, a storage cappacity of 40 TB, and a high speed 10 GB/s internet conexion; within the Grid component of the Center the grid site Ro-14-ITIM has been certified.

The good results obtained in the last four years by the teams involved in research and development are also due to an efficient cooperation with the technical support teams on one side and the administration staff of the institute on the other side. The institutional management has undertaken a profound improvement in the last years – the most significant achievement is the implementation and certification of an ISO 9001:2008 quality management system combined with an integrated economic management system.

This brief presentation of the institutional component, and of the major achievements of INCDTIM in the last four years will be followd by the self-assessement reports of the all 13 research teams.

2.2. Activity report by team

Self-Assessment Report: Team E1 - Structural determinations of molecular compounds by mass spectrometry and chromatography

Members: Zaharie Moldovan (SR I), Cezara Voica (SR III), Veronica Avram (SR) Florina Tusa (SR), Olivian Marincas (SR), Kovacs Melinda (SR III), Schmutzer Gabriela (SR), Feher Ioana (RA), Curean Ioana (Th), Olteanu Simion (Th), Olteanu Sorin(Th). The group have: 1 SR I, 2 SR III, 4 SR, 1 RA si 3 technicians. Among researchers 3 have doctor title and 5 of them are candidate for a doctor degree.

Quality of the research activity

Published papers: From 2007 the group have published 31 papers, where 19 are ISI papers, accumulating an influence scor of 10.72 and 20 citations. A number of 14 papers were published in colaboration with autors from european institutes (Switzerland, Germany, Spain).

Reprezentatives papers: A28, A48, A209, A213, A235, A288, A293, A303, A319, A383.

Scientific conferences participations: The group members have been participated at **87** national and international scientific conferences (5 are as invited conferences).

National and international projects:

From 2007 the group participated at 13 projects: 11 national projects (5 as Coordinator and 6 as Partner), 1 as EU-FP6 and 1 as a bilateral cooperation (CF6, CF7, F22, F24, F25, F27, F52, F73, F75, F76, F89, F90, F106)

Main Research Field:

a) Levels and fates of organic pollutants in natural waters (A48, A209, A235, A303, CF7, F24);

b) Investigation of pollutant removal processes from water medium (A288, A383, F25, F75, F76, F106)

c) The modern methods for investigation of pictorial materials from art objects (A213, CF6);

d) Structural investigation of the pharmaceutical products by mass spectrometry (A28, A293, A319)

e) Advanced methods for determination of sweeteners and colorants in drinks for quality assurance and food security (F73, F90)

Patent request

Invention title: Catalytic mineralization process of organic contaminants from rezidual water, Patent Number(s): RO122840-B1, Assignee: UNIV CLUJ-NAPOCA BABES-BOLYAI, Inventor(s): COSOVEANU V; DANCIU V; MOLDOVAN Z, et al.

Other activities

An important activity of the group is the development of methods for solving requests from economic units. The aim of this activities was to identify the structures of new sintetized materials or detection of the trace of compounds in complex substances. In our group a number of 10 methods are accredited, in accordance with ISO 17025 (*Mass Spectrometry, Chromatography and Ion Physics* Laboratory Certificate Number RENAR Nr. LI 823/2009). and are grouped in two categories:

A) Determination of organic indicators by chromatography and mass spectrometry (9 methods);

B) Determination of metals traces by ICP-MS (1 method).

Human resouces quality

The research group "Molecular structures by mass spectrometry" consists of 11 members having different specialties (as physicist, chemistry, engineer and technicians) being in the category form of young researchers, the **average age** of the team is **37** years. Among researchers 3 have doctor title and 5 of them are candidate for a doctor degree. In the last years the group structure changed due to the entry of young researchers in the group.

Competencies of the team

The members of research team are highly qualified, with few of the researchers participations in international research programs and scientific cooperation. The group skills with application at molecular structure determination are:

1. Exact mass determination by high-resolution mass spectrometry;
2. Study of molecular fragmentation under electron impact;
3. Mechanism of production of ions by ion-molecule interaction;
4. Kinetic energy release in the fragmentation processes;
5. Application of isotopic labeled methods in structural elucidation;
6. Application of hyphenated techniques to determination of molecular structures.

International experience of personell

Dr. Zaharie Moldovan. a) Instituto de Recursos Naturales y Agrobiología de Sevilla, Spania (1.11.1992-30.10.1993): Mass spectrometry applications in soil organic matter determinations; b) University of Seville, Spain (1.11.1993-31.12.1995): Molecular degradation under biological and

chemical agents (Project EU "Integrated Chemical and Biological Treatment of Industrial Wastewater", EV 5V-CT93-0249); c) Institute for Chemistry and Environmental Investigations from Barcelona (IIQAB), (1. I. 1999-31. V. 1999): Molecular extractions from complex matrices using supercritical fluids method; d) Institute for Chemistry and Environmental Investigations from Barcelona (IIQAB) (1. XI. 2000-30. IX. 2001): EI-MS and CI-MS as complementary methods at molecular structures determinations; e) EAWAG, Zurich, Elvetia (iulie 2007): Samples preparation methods.

Dr. Melinda Kovacs. a) Second French Serbian Summer School: "Water quality control – from concept to action" Vrnjacka Banja, Serbia, Octombrie, 2007; b) European Institute of Membrans, Montpellier, France, October – December, 2007; c) Summer school: Health Risk Assessment – principles and applications, Karolinska Institute, Stockholm, Sweeden, April 2008 and June 2010.

Drd. Marincas Olivian: BfG Koblenz, Germany: Determinations of poluttant adsorbtion constants.

Scientific journal reviewers or doctor degree board

Dr. Zaharie Moldovan is reviewer at *International Journal of Environmental Analytical Chemistry, Journal of Environmental Monitoring, Chemistry and Ecology and Chemosphere* and doctor degree board member at „Babes-Bolyai" University and „Iuliu Hateganu" Medicine University from Cluj-Napoca.

Research topics which will be developed in the next stages

In the next stage will be boarded especially interdisciplinary research based on high performance mass spectrometry and chromatography, which on medium and long term should lead to a sustenable development. It will be focused on problems of environment and food safety that potential will help at:

(a) environment remediation;

b) studies on climatic changes on environment quality;

(c) product food authentification and control;

(d) research activities focused to economical activity stimulations;

(e) research activities focused to national products promovation in european markets.

Based on group capacity of cooperations with international parteners will be boarded research from European Programme.

Infrastructure quality

High resolution mass spectrometry (HRMS); Coupled system gas chromatograph - mass spectrometer (GC-MS); High pressure liquid chromatography (HPLC); Inductived Cupled Plasma - Mass Spectrometer (ICP-MS).

Next stage development: mass spectrometer of high resolution and sensitivity from ORBITRAP class.

Self-Assessment Report: Team 2 – Stable isotope applications group

Team: Dana Alina Magdas, PhD (CS III), Gabriela Cristea, PhD (CS III), Adriana Dehelean, PhD (CS III), Romulus Puscas, , PhD student (CS), Zoltan Balazs, PhD student (CS), Phys. Edina Dordai (CS), Eng. Mirel Valentin (IDT II), Tech. Nicoleta Petrica, Tech. Stelian Radu.

The quality of research activities

The main research fields of the team are:

- Authenticity and traceability of food and beverages (wine, honey, fruit juices)
- Isotopic hydrology research: water origin assessment, recharge mechanism, efficient management of water resources
- Using the stable isotopes in the study of the global carbon cycle
- Plant physiology – isotopic fractionation of the carbon, oxygen by plants
- Isotopic geochemistry
- Isotopic characterization of CH_4 at natural concentration and natural isotopic abundances

In the last 4 years, the team members have published: **17 ISI articles,** the relative influence score of these being **26.428** and other **5 ISI articles,** with no calculated impact factor. The published articles in last four years have generated **46 citations in ISI** journals. Other **4 ISI articles** are now **in press**, their total influence score being 2.2. There are also **9 articles** submitted to **ISI journals**.

Beside ISI articles, the group members had published in the mentioned period **11 non ISI articles** and **2 books**. The obtained results were presented at different scientific events both national and international, as: invited lectures, oral and poster presentations (**54 international conferences** and **12 national conferences**).

National funding projects in which team members were involved: a) INCDTIM-**cordinator**: **1** project **RU-TE, 4** projects **Parteneriate type, 2 CEEX** projects; b) INCDTIM – was partner in **7** projects. Due to the interdisciplinary themes addressed in these projects, most national projects carried out were performed in collaboration with colleagues working in other research groups within the institute.

Besides the Romanian research parteners, our group had very intense collaborations with research groups from abroad, like: Austria (*Austrian Institute of Technology*), Hungary (*Institute of Nuclear Research, ATOMKI, Debrecen*), Switzerland (Institute *of Mineralogy and Geochemistry, University of Lausanne, Switzerland*), France (*Paris-Sud University, ESE-CNRS, France*), Spain (*Complutense University, Madrid*). These collaborations consisted both by joint research projects and by joint research articles. Thus, in last years our group was involved in two bilateral-

cooperation projects: Romania – Hungary (F105) having the topic: *Applications of stable isotopes in study food and water quality* and Romania – Austria with (F108) the topic *Isotopic composition of river waters in the Danube basin*. Another bilateral project Romania – Austria ("*Application of advanced methods in determination of geographic origin of wine: comparison of Austrian and Romanian wine")* was evaleted and will be financed starting 2012. In partnership with the colleagues from abroad, the group members have published in last years three articles: 1**ISI article** is in print and other **2 ISI articles** are in preparation.

Most of the group members belong to Accredited Laboratory of "*Mass Spectrometry, Chromatography and Ion Physics*" (Certificate Number RENAR Nr. LI 823/2009). In the frame of this laboratory, the RENAR accredited a method of "Determination of isotopic ratios ($^{18}O/^{16}O$; $^{13}C/^{12}C$) from wine" that allowed us to gain economical contracts. Thus, we transferred to economical environment not only the know-how related to the method of the isotopic analysis of wine, but also our expertise gained in the development of different research projects. The most important beneficiaries of our expertise related to isotopic fingerprint of wines: Ministry of Agriculture and Rural Development; A.N.A.F.; D.A.D.R. Vrancea; The wine branch organization Viti-Vinicola; S.C. Vinton SRL, Galati; S.C. Cotnari, S.A.; S.C. Vincon Vrancea, S.A.; S.C. Prodvinalco, S.A.; S.C. EuroProd TGB, S.R.L.

The laboratory of "*Mass Spectrometry, Chromatography and Ion Physics*" because of the accredited method of "Determination of isotopic ratios ($^{18}O/^{16}O$; $^{13}C/^{12}C$) from wine" was declared approved laboratory by the Ministry of Agriculture and Rural Development, for performing isotopic analysis in wine authenticity control. Moreover, starting this year, our group performs the isotopic measurement ($^{18}O/^{16}O$; $^{13}C/^{12}C$) of Romania's authentic wines. It is important to mention that until the method was implemented in our laboratory, these measurements were performed in the European Commission laboratory from Ispra and 2011 is the first year when these analyses were performed inside the country, in our laboratory. For these reasons, an important aspect of our activity is the quality control of our experimental results. To fulfill these requirements our group is participating on a regular basis at different proficiency tests. The last proficiency test in which our team had participated, obtaining very good results, was organized by International Atomic Energy Agency, IAEA, Vienna.

The developed isotopic methods which are use in our group (isotopic analysis for carbonate, organic matter, mineral waters) allowed us to obtain economical contracts. We mention here only some of our most important customers: Geologic Institute of Romania (economical contracts of about 16.750 lei); University of Agricultural Science and Veterinary Medicine, Cluj_Napoca (economical contracts of about 22.250 lei), companies (National Company of Mineral S.A. Bucureşti; Romaqa Group Borsec; S.C. Jacon-Tex S.R.L. Reghin; S.C. Apemin Tusnad S.A.; S.C. MIOMIL S.R.L.; S.C. CARPATHIAN PLASTICS CORPORATION S.A.).

Another activity in which our research group was involved was to make popular and disseminate at large scale the obtained ressults related to climate changes. For this, we have participated, as associated partners at the FP7 European Project CarboSchools http://www.carboeurope.org/education/.

The human resources quality

The research group "Stable isotope applications group" consists of 9 members having different specialties (6 physicists, 1 engineer and 2 technicians) being form mainly by young rese archers, the **average age** of the team is **37** years. From this, **3** persons have a PhD and 2 are PhD students.

In the last years the group structure changed on one hand due to withdrawal of three prestigious scientists by retirement, on the other hand due to the entry of young researchers in group.

Group members received doctoral and master research internships at different important European Universities: Dr. Dana Alina Magdas*, "Marie Curie" scholarship at Complutense University from Madrid, Spain*; Dr. Gabriela Cristea*, master scholarship at Claude Bernard University, Lyon, France*; Fiz. Edina Dordai*, master scholarship at Gent University, Belgium*). Beside these, team members had participated at different trainings and summer schools: **Dr. Dana Alina Magdas**: ***2*** *trainings at Complutense University, Spain;* ***1*** *training at Karlsruhe Institute, Germany;* ***1*** *summer school at Munchen University, Germaniy;* ***1****summer school at Vienna University, Austria*; **Dr. Gabriela Cristea**: ***1*** *research stage at Istituto Nazionale di Fisica Nucleare, Italiy*; ***1****summerschool at Vienna University,* ***1*** *training, Budapest University, Hungary).*

New research topics

1. Isotopic fingerprinting of Transylvanian fruits (Current Project: RU-TE: 120/2010)
2. The extinction of our isotopic methods for authentication of meat and milk products
3. Development of complementary isotopic methods which allow the distinguish between organic and traditionally cultivated fruits and vegetables
4. Application of isotopic methods in Danube waters studies, as indicator of climate changes

Self Assessment Report Team 3: „Carbon Nanostructures and Hydrogen Storage"

Membership: **CSI Phys. Dr. Biris Alexandru**; CSI Chem. Dr. Lupu Dan Miron; IDTI Eng. Coldea Ioan; IDTI Eng. Misan Ioan; IDTI Eng. Toma Ioan; CSIII Chem. Dr. Blanita Gabriela; Chem. drd. CS Ardelean Stefania; Chem. drd. CS Ardelean Ovidiu; Phys. AC Biris Gabriela;

The research activity is focused on two main areas having as a strategic objective the **research and development of advanced materials and innovative methods** that can result in competitive products and services and technology transfer.

(a). Hydrogen storage, started in 1975, as part of the National Hydrogen Program by the multidisciplinary team „Metal Hydrides and Applications". Many compounds have been prepared and intensively studied: intermetallic compounds, complex hydrides of light elements, amides and amide-hydrides combinations, the major focus being the improvement of the hydrogen storage and absorption/desorption kinetics in order to develop applications in: electrochemical hydrogen storage in metal hydride electrodes for Ni-MH batteries, development of a thermal compressor for ultra-pure hydrogen for fuel cells and hybrid vehicles and of a thermal engine based on hydrogen absorbing metal alloys that used solar energy or residual energy. Currently, the research team is involved in the study of metal-organic frameworks and composites of carbon based catalysts.

b) A new research direction of the team developed since 2004, has been the **synthesis and characterization of carbon nanostructures** (nanotubes and nanofibers) and their use as hydrogen storage materials and other advanced applications. For the first time in the world, there was accomplished at INCDTIM the synthesis of carbon nanostructures based on the CCVD method with inductive heating [*Carbon*, **42**(3),503-507, 2004]. This method allows the growth of carbon nanostructures of superior quality as compared to the classic CCVD with thermal furnace *Chem.Phys.Lett.***429**,(2006),204-208].

In the last few years, we focused on the improvement of **synthesis and purification of single- and multi-wall carbon nanotubes** and their use in bio-medical applications (partner in 3 PNCD II-2007-08 projects). Additionally we focused on the controlled synthesis of graphenes (discovered in 2004) over metallic catalysts (Fe, Co, Mo) and oxide support (MgO) (publications A 168 and A 305 from the INCDTIM list) and the direct synthesis of graphene sheets with noble metal nanoparticles encased in their graphitic structure over Au, Ag, Pt catalysts supported on MgO (publication A 287 from the INCDTIM list). These studies represent another two world first-time technologies, and which resulted from our collaboration with the *Nanotechnology Center, University of Arkansas at Little Rock, USA.*

Quality of the research activity

- Between 2008-2011 the team published **46 peer-reviewed publications ranked ISI,** with a **cumulative relative impact score of 101.96 (the average relative impact score per publication was 2.21).** All these **46** publications have been developed in collaboration with foreign scientists. **31** publications **have been cited 302** times, representing an average of 10 citations/publication. The most important citing papers are: *Nature Nanotechnology* [**4**(1), 64, 2009.] (**A48** from the list) and in *Nano Letters* [**8**(5), 1417, 2008 and **9**(5), 1866, 2009] (papers A 35 and A 48)

- **1 book chapter published**

- **29 presentations/participations** at national and international conferences

- The members of the team participated in **14 national research** projects competitively won and as a Director/Project Coordinator in **4 projects** (**CF 5, F 23, CF 47, CF49**) and as a Project Partner in **10 projects**(**CF 8, CF 9, CF10, F37, F38, F 64, F67, F 78 F107)**

- **3 USA patents; - 1 USA patent application; - 4 patent applications with OSIM**

Quality of the human resource

The team involves 9 members (3 PhD, and 2 PhD students) of complementary specializations: physics, chemistry, engineering.

Technical Competencies of the team:

Synthesis and characterization of the carbon nanostructures.

Synthesis and characterization of hydrogen absorbing materials (intermetallic compounds, complex hydrides of light elements, amides and amide-hydride combinations, metal-organic frameworks and composites of porous carbon structures);

Study of the thermodynamic and kinetic aspects for the hydrogen adsorption/desorption in solid materials. These applications were focused on technologic transfer;

The research team is highly qualified, with few of the researchers participating in international research programs and scientific visits: **Dr. A. R. Biris** – is Scientific Affiliated Researcher to the University of Arkansas at Little Rock, Nanotechnology Center, AR, USA; **Dr. Dan Lupu** – Research guest of the Fribourg University, Switzerland, **Eng. Ioan Misan** – technical preparation visit at the European Organization for Nuclear Research –CERN, Geneva, Switzerland.

Activities as reviewers in specialized peer-reviewed Journals:

Dr. Dan Lupu: Journal of Optoelectronic and Advanced Materials; International Journal of Hydrogen Energy; Recent Patents on Engineering Bentham Science Publishers; Carbon and Journal of Vibrational Spectroscopy. ***Dr. Alexandru Biris***: Materials Research Bulletin, Particulate Science and Technology Journal. ***Drd. Stefania Ardelean***: ACS NANO

Collaborations and partnerships with other national and international institutions:

National research partnerships: National Institute for Materials Physics – Bucharest, "Babes-Bolyai" University - Cluj, "Iuliu Hatieganu" University of Medicine and Pharmacy - Cluj, "Horia Hulubei" National Institute for Physics and Nuclear Engineering-Bucharest.

International partnerships: University of Fribourg, Switzerland; University of Rostock, Germany, HSCH Wismar, Germany, Energy Technology Research Institute, Tsukuba, Japan, IFW-Dresden, Germany, University of Arkansas at Little Rock, USA, Institute of Physical Chemistry, National Centre for Scientific Research "Demokritos", Athens, Greece

Infrastructure quality and its degree of exploitation

1. Installations designed and built within INCDTIM Cluj-Napoca: installation for the synthesis of carbon nanostructures by CCVD with Inductive Heating (50%), Sievert-type installation for the characterization of the hydrogen absorption/desorption thermodynamics and kinetics (>70 %);
2. New equipment purchased in the last 4 years: Raman spectrometer (>70%); thermogravimetric analysis (>70%), UV-VIS-NIR spectrophotometer (50-70%);
3. Scanning (SEM) and transmission (TEM) electron microscopy was performed in bilateral collaboration with the Nanotechnology Center of the University of Arkansas at Little Rock, Arkansas, USA.

Perspectives

By winning 2 research projects in the PN-II-IDEI 2011 competition for the following period (until 2014) the team is involved in the following research activities:

(a) Synthesis and purification of graphene sheets with metal nanoparticles of Au and Pt encased in their crystalline structures with the focus on their utilization in electrochemical oxidative studies of DNA (PN-II-ID-PCE-2011-3-0129)

(b) Study and evaluation for the improvement of the H_2 absorption by using the spillover method in MOF-composites with supported catalysts (PN-II-ID-PCE-2011-3-0350). New methods for the synthesis and purification of MOFs with high surface area for hydrogen cryo-adsorption; nanoconfinement of materials with high storage capacity of hydrogen in porous structures in order to improve the thermodynamic and kinetic characteristics, as requested by mobile applications.

There have been submitted 2 project proposals: (1) "Hydrogen storage in novel nanostructured metal doped carbon materials" along with Dr. T Steriotis (Institute of Physical Chemistry, National Centre for Scientific Research "Demokritos", Athens, Greece) as part of the bilateral collaboration Greece-Romania; (2) "Material World Network: Development of Non-precious Metal-based Cathod Materials" along with Dr. A.S. Biris (University din Little Rock, Arkansas, USA) as part of the bilateral collaboration USA-Romania.

Self-Assessment Report: Team 4 - High-Tech Engineering in ATLAS Experiment at LHC CERN Geneva

Group leader: Engn. Gabriel POPENECIU

This team is a part of the Romanian ATLAS group which includes experimental and theoretical particle physicists as well as electronic, mechanical and information technology engineers. We participate at the international ATLAS Collaboration, as Romanian entity, together with another 4 Romanian institutes/universities, in 2 Memorandum of Understanding between CERN and Romanian Funding Agency for: (i) Construction of ATLAS Detector (1998) and (ii) Collaboration to provide computing power and storage capacity to Worldwide LHC Computing Grid (2006).

ATLAS detector includes Tile Calorimeter subdetector, consists of 3 hadronic calorimeters with scintillating tiles for the measurement of hadron energy. The researches of our group were involved as co-authors in the ATLAS Collaboration for some basic Tile Calorimeter's papers which are fundamental for the subdetector design and construction: ''ATLAS Calorimeter Performance - TDR", "ATLAS Computing- TDR" and ''Tile Collaboration, Design, Construction and Installation of the ATLAS Hadronic Barrel Scintillator-Tile Calorimeter ATL-TILECAL-PUB-2008-001.

In the period 2007-2011, during 2007-2008 our group was mainly involved to bring into functional parameters the Tile Calorimeter; and 2009-2011, in the frame of ATLAS collaboration, the responsibility moved to detector operation and maintenance, and to finalize the commissioning phase and our R&D activities are strongly correlated to these aims.

I. Topic of research and main results (2007-2011)

(i) Contributions to the construction and commissioning of the Hadronic Tile Calorimeter

The contribution of the group to the construction of the Tile Calorimeter, has been a significant one from the beginning until the end of the construction. The mechanical team, starting with 1996, have been in charge with the design and validation of all the pieces constructed in Romania, to the assembly of the modules on the surface and in the pit, in the large barrel and in the two extended barrels. The electronic team was responsible on cabling, inserting of optical fibres inside modules, optical instrumentation, tests of the Front End electronics.

Results: - Elaboration of the Procedures ''*Extended Barrels Movement – Work Plan*" (CERN-Atlas code ATL-HT-OP-001);

- Contributions to bring into functional parameters the Extended Barrels, EBA and EBC;

- Elaboration of the procedure and technical design for special devices for the EBA and EBC, movement in the working position;

- Commissioning of the Tile Calorimeter, measurement, repairs and testing of the electronic units (drawers), using MOBIDICK data acquisition system.

(ii) Contributions to ATLAS Tile Calorimeter Maintenance

Our team are taking part permanently to maintenance activities during LHC technical stops. Repair of the damaged electronics drawers and the replacement of the bad Low Voltage Power Supplies (LVPS) are the main tasks which will be finished in 2013 LHC long shutdown.

***Results*:** - Development of the CERN-INCDTIM project ''*Tile Calorimeter Basket Engineering''*. The objective was to design a system that allows to withdraw the drawers from Tile Calorimeter modules permitting electronics repair in situ. The special device designed and constructed in our institute was validated at CERN and now is used in all the maintenance procedures for super-drawers manipulation;

- Drawers refurbishment during first LHC Machine shut down: repairs of Tile electronics drawers and LVPS replacement using special device developed by INCDTIM Cluj.

As a result of the excellent performance and operation of the experiment, as well as the superb performance of the machine, ATLAS has recorded an integrated luminosity of 5.2/fb with stable beams, corresponding to an overall data-taking efficiency of 93.5%.

(iii) ATLAS Tile Calorimeter Upgrade

The participation of the Romanian group in the ATLAS experiment upgrade is described in "*TileCal phase II upgrade R&D program*" ATLAS Project document. Our group is involved in R&D activities in the WP2 *On-detector electronics*, WP 5 *Evaluate alternative drawer mechanic solutions* and WP 6 *Installation*.

***Results*:** - Contributions to evaluate alternative drawer mechanic solutions, to assure an easier service and to have electronics more accessible. The proposed design divides the drawers into mini drawers of half the size of the standard drawers.

- Study of Tile Calorimeter electronics replacing and testing: the task: ''full readout of all Tilecal data'' is driven by radiation tolerance, aging and the need for additional information to L1Calo to keep L1 rate below 100 kHz. We are involved in some different R&D projects which explore detailed solutions and after their testing a final solution will be applied to a prototype drawer to be tested during 2013 and 2014.

(iv) Grid Activity

As a member of Tier 2 Romanian Federation governed by a MoU for LCG (**L**HC **C**omputing **G**rid), we design and developed a GRID site, ***RO-14-ITIM***, which is integrated in Tier 2 Grid Federation Center and performs computations in ATLAS VO.

***Results*:** - R&D for the configuration of RO-14-ITIM site: hardware support, operation system and software.

- Site maintenance, operation and management according to ATLAS requirements;
- Soft and hardware upgrades according to ATLAS requirements and financial resources.

II. Quality of the research activity

Papers in ISI ranked journals: total **56** papers, out of which: **53** as co-authors of the ATLAS Collaboration and **3** as main authors. The most relevant journals in which the papers were published: *Physical Review Letters, Physics Letter B, Journal of High Energy Physics, Physics Review D* and *Nuclear Physics B.*

- The cumulated relative influence scores for all the publications is **179.50** (average of **3.20/paper**).
- Number of citation: **182**

Papers in non-ISI journals: **10**

Major international scientific meetings attended: **22**; ATLAS Collaboration Weeks 2009 – 2011, Tile Calorimeter Weeks 2007-2011, ATLAS Upgrade Weeks 2010-2011, XXIII International Symposium on Nuclear Electronics & Computing, NEC 2011, Annual Meeting of the Romanian Tier-2 Federation 2007-2011.

Coordinated projects: total **9** projects from peer-reviewed competitions, out of which **8** are financed from national research programs, and **1** from EU Structural Funds (position F29, F39, F42, F94, F103, CF18, CF19, CF34, respectively F111, in the INCDTIM Cluj Napoca projects list). For the period 2007-20011, these projects were funding with a total of **1,075,000** euro.

III. Available infrastructure

- Data Center infrastructure with our Grid system for RO-14-ITIM site (position no.1 in the equipment list of INCDTIM).
- Institute Prototypes Workshop

IV. Perspectives for future developments

To continue the R&D activities in ATLAS Collaboration and in LHC Computing Grid, together with our Romanian partners, we applied with 2 projects to the Programm ROMANIA-CERN, evaluated by the International Scientific Advisory Board (ISAB). These 2 project with a total value of over ***450,000 euro***, for the next 3 years, will provide a good environment to reach our aims: ***to give a strong support for operation and upgrade of ATLAS detector; to maintain and operate processing infrastructure; and to increase competitiveness, contribution and visibility of our group.***

Self-Assessment Report: Team 5 - Nanocomposites materials with tailored properties

Group Leader: Dr. Ioan-Ovidiu Pana;

The group was formed since 2007 by gradually bringing in various researchers into an initial core consisting of Dr. Ovidiu Pana, Dr. Maria - Loredana Soran, PhD student C. Leostean and engineer Sergiu Macavei. As the research directions of the group became better defined, especially in the field of magnetic nanosystems with tailored properties, due to existing convergent research areas, into the group was integrated the electron paramagnetic resonance (EPR) group (4 persons). Other trained researchers originating from other teams or from outside the institute were integrated as weel as the activities were focused on new types of nanocomposite materials with biomedical applications. The resulting group has an interdisciplinary character being composed from physicists (7 persons), chemists (5 persons), one physical – chemist, one engineer and one technician. By scientific degree: the team contains CS I-1 pers., CS II-2 pers., IDT II-1 pers., CSIII-5 pers., CS - 2 pers. The average age of researchers is 37 years. **Large equipments utilized**: chemical synthesis laboratory, X-ray diffractometer (Bruker 2008), equipment XPS (SPECS 2008), magnetometer VSM "cryogen free" (CRYOGENIC 2007), SQUID magnetometer (Quantum Design 2008), microscopy AFM / STM - UHV (RHK 2008), HPLC with accessories like mass spectrometer (Shimadzu 2008).

The main research topics of the team are as following: **(1) Magnetic Nanocomposites with adjustable magnetic features and predetermined architecture, composition and bio-functionalization**. The topic is focused on synthesis and characterization of composite nanoparticles containing superparamagnetic or hard magnetic materials, polymers, noble metals. By studying magnetic nanoparticles coated with doped oxide semiconductors based external shells one can obtain predetermined luminescent properties. Generally, by using various types of complex multifunctional nanoparticles one can develop important applications for the detection and separation of biomolecules and for cell targeting in biomedicine; **(2) Nanoparticles based on magnetically diluted oxide semiconductors**. The topic is focused in synthesis and characterization of magnetically diluted nanostructured semiconductor materials doped with 3d ions. Magnetic properties, electrical, structural and spin dynamics of such nanoparticles are investigated; **(3) Methods and materials used for studying of organic compounds from different matrices and nanosystems**. The main objective is to determine the organic compounds inserted in various matrices and nanosystems by using different extraction methods associated with chromatographic and spectrophotometric analysis; **(4) Nanosystems with photo-electrocatalytic properties.** It reefers to the characterization, testing and applications of the oxides nanosystems with photocatalytic properties**.**

Main collaborations and partnerships. **National***: Natl. Inst. R&D for Mater. Phys*. Bucharest, *Faculty of Phys*. Babes-Bolyai University of Cluj-Napoca*, Faculty of Material Eng. and Environment* of Tech. Univ. Cluj-Napoca, *Nanomedicine Dept*. from Univ. of Medicine and Pharmacy of Cluj. **International**: *Institute des Materiaux Jean Rouxel,* Nantes, France*; Institute of Polymer Science and Technology*, ICTP, CSIC Madrid, Spain*, Institut fur Physikalische Chemie,* Universitat Stuttgart, Germany.

Ongoing activities and results. Outstanding results correlated with immediate activities regarding nanocomposite materials are: **(i)** synthesis and characterization of nanoparticles with different magnetic cores covered with multiple coatings based on Fe, Pt, conjugated polymers (especially polypyrrole - Ppy), silica and / or TiO_2; the objective is to investigate the effects of core-shell structure formation when different architectures, based on multiple components, are used for the formation of nanoparticles with adjustable magnetic and dispersive properties; different functionalizations are realized in order to obtain pre-defined properties demanded by various applications; (*Core-shell composite nanoparticles based on Fe and Pt having adjustable magnetic dispersive and functional properties*, project IDEI- 2011, 2011-2014, pr. man. O. Pana); **(ii)** synthesis and characterization of new composite core-shell nanoparticles of Fe_3O_4@ZnS and Fe_3O_4@TiO_2 type with predetermined magnetic, structural and luminescent properties (foreseen applications in medicine and biotechnology); (*Composite core-shell nanoparticles based on magnetite and semiconductors with predetermined properties*, project PD 2011 pr. man. Maria Stefan); **(iii)** study of interfaces in magnetic nanoparticles systems having a core-shell structure; fundamentals concerning interaction effects at the interface between the iron magnetic cores and Au or Pt external shells; evidence and control of charge transfer from coating polymers to the surface of magnetic nanoparticles; (*Surface and Interface Science: physics, chemistry, biology, applications,* project "Complex Ideas", ID_76/2010, 2010-2013, resp. O. Pana, coord. INCDFM). Current activities in the field of magnetically diluted semiconductors: by using both XPS and EPR techniques the effects of 3d transition ions doping of nanoparticles and thin film composed from oxide semiconductors such as $Zn_{1-x}TM_xO$ and $Ti_{1-x}TM_xO_2$ (TM = Mn, Fe, Co) are under investigation; there were evidenced changes the of magnetic, structural and morphological properties as well as modifications of the spin dynamics correlated with the reduction of particle sizes or thickness of thin films; (*The effects of doping and of dimensionality on magnetic properties, structural and morphological and spin dynamics in ferromagnetic oxide micro and nanostructures*, project "Complex Ideas", ID_106/2010, resp. O. Raita, coord. UTCN). Ongoing studies on photocatalytic nanomaterials refers to the synthesis and structural characterization (Raman, ESR, FT-IR, XRD) of nanostructured oxide materials and coatings based on TiO_2, mixed oxides, doped calcogenides; determination of their specific photocatalytic properties, especially in hydrogen production area, is also under investigation;

Additionally the effect of microwaves fields, as stress factor, at different intensities to the content in essential oils, vitamin C and secondary metabolites (BVOC) from indigenous plants. (*Effects of microwave fields on essential oils and secondary metabolites of some indigenous plants*, project TE 2011, 2011-2014, pr. man. M.-L. Soran);

Involvement in international projects*: N*etwork of Excellence „Nanostructured and Functional Polymer Based Materials and Nanocomposites - NANOFUN-POLY (FP6 2005-2008); 'Hybrid systems basen on polymers and magnetic nanoparticles ("Brancusi" type bilateral project 2009-2010).

Future foreseen developments. In the near future our team intends to focus its research activities towards the applications of nanostructured systems in biology and medicine. The exact formulations of the future research targets result from the following project titles newly submitted to CCCA 2011 competition: **(1)** *Core-shell nanoparticles as bio-conjugate platforms in cancer cells targeting and therapy* (Ovidiu. Pana, CS I); **(2)** *New highly efficient TiO_2 based photo-catalytic systems for biomedical applications* (Emil Indrea, CS I); (**3**) *Antibiotics determination from environment and their effects on microbiota and nutritional plants* (Maria L. Soran, CS II); **(4)** *Multifunctional nanoparticles with adequate properties for controlled drugs delivery and release* (Maria Stefan, CS III); **(5)** *Multicomponent nanoparticles with magnetic, optic, dielectric and functional properties used for detection of biomolecules* (Adriana Popa, CS III). In the next years our team also intends to realize the implementation of a complex deposition system of organic-inorganic composite thin films by using atomic layer deposition, layer by layer deposition, organic layer deposition, chemical vapor deposition and pulsed laser deposition methods with applications in biomedicine, molecular sensors, photovoltaic cells, storage information, etc.

Scientific publications and communications of our team in the period 2007-2011can be summarized as following: **(1)** a total 40 ISI articles with 36.38 cumulative relative influence score; 11 of these articles have co-authors from aboard; **(2)** 4 Books; **(3)** one national patent; **(4)** 15 unrated ISI articles; 6 articles published non ISI listed journals; **(5)** 12 invited lecturers and seminars; (**6)** 142 presentations at international conferences.

Self-Assessment Report: Team 6 - Functionalized hybrid materials based on polymers and inorganic nanoparticles

Group leader: Dr. Rodica Turcu

The research activity performed by the team is part of a highlight topic area related to the development of the new nanotechnologies and advanced nanostructured systems with controlled functionality having great applicative potential. The multiresponsive nanocomposites are the subject of intense researches worldwide motivated by promising applications in biotechnologies and nanomedicine and therefore the activity of our team focused on the following research topics:

a) **Innovative methods for synthesis of polymers with special properties and hybrid materials polymers / magnetic nanoparticles.** The significant results consist in the development of the following original methods: (i) Synthesis method of hybrid nanostructures based on magnetic fluid and functionalized polypyrrole; (ii) Synthesis method of magnetic nanoparticles in ionic liquids as reaction medium; (iii) Microwave assisted synthesis method of hybrid nanostructures based on magnetic nanoparticles and polylactones; (iv) Synthesis method of intelligent hybrid materials based on magnetic nanoparticles and polymers /copolymers responsive to external stimuli (core-shell systems, macro and microgels).

b) **Functionalized hybrid materials polymers / inorganic nanoparticles.** The preparation of new functionalized hybrid materials based on polymers requires as a first step the synthesis of functionalized monomers and therefore a part of the research activity focused on this issue. The original results obtained by the team are the synthesis of pyrrole monomers and new derivatives of acrylic acid with attached functional groups (carboxyl, aminoacids, polypeptides).

New functionalized hybrid materials with controllable properties by molecular architecture and nature of the components were obtained: (i) Hybrid nanostructures based on magnetic nanofluid and functionalized polypyrrole; (ii) Core-shell type hybrid nanostructures based on magnetite and biocompatible polymers (poly-caprolactone, poly-lactic acid, poly-hydroxyethyl methacrylate, poly N-isopropylacrylamide); (iii) Intelligent hybrid materials with stimuli responsive properties based on magnetic nanofluid and responsive polymers (poly N-isopropylacrylamide, poly- acrylic acid) – magnetic macro and microgels; (iv) New recyclable organic catalysts based on functionalized magnetic nanostructures.

c) **Characterization and assessment of applications of functionalized hybrid materials.** The characterization of the functionalized hybrid materials was performed using various techniques either available in INCDTIM: XRD, DLS, XPS, magnetic measurements (VSM, SQUID), or in other institutions in the framework of national and international collaboration: TEM, HRTEM. It is worth mentioning a new research initiative of the team regarding the investigations of magnetic hybrid nanostructures as core-shell and microgel type by Small Angle Neutron Scattering (SANS)

method – Application for beam time accepted at Budapest Neutron Center, Hungarian Academy of Sciences 2010.

The research activity focused on the assessment of applications of functionalized hybrid materials for magnetic separation of proteins and biomolecules of interest in the pharmaceutical industry. The experiments were performed in collaboration with the foreign partners in the framework of the project FP7 MagPro2Life, the team E6 being involved as a partner into this project. ***The tests of magnetic separation of biomolecules using the magnetic microgels produced by our team were performed by the FP7 project partners (MERCK, Karlsruhe Institute of Technology) and demonstrate that these materials have very good properties suitable for magnetic separation application.*** Our team prepare magnetic microgels (hundreds of grams quantities) required by foreign partners for testing in magnetic separation pilot lines.

Another applicative research topic of the team is the assessment of application of functionalized magnetic nnaostructures as new recyclable organic catalysts for different chemical reactions (Aldol reaction, Michael addition, etc.) which have significant impact in chemical, pharmaceutical or cosmetic industry.

Recently, the team approached ***a new interdisciplinary research topic*** related to the ***applications of magnetic microgels in nanomedicine as new nanocarriers for targeted drug release***. The assessment of this application will be done in the framework of a signed *Collaboration Agreement between a prestigious institution from abroad Universitätsklinikum Erlangen - Section for Experimental Oncology and Nanomedicine(SEON) Erlangen, Germany and two Romanian institutions INCDTIM and Romanian Academy-Timisoara Branch.*

The results of the research activity were published, presented at scientific meetings and included in patents applications. The activity of the research team was appreciated by the international scientific community, this team being involved as an active partner in 2 international projects financed by the European Community: FP6 NANOFUN-POLY 2004-2008 and FP7 MagPro2Life 2009-2013.

10 articles were published in ISI journals, 7 articles in other journals and 4 book chapters published abroad. We mention that from the 17 published articles, *9 articles have co-authors our collaborators from abroad.*

The articles were published in the following journals, having **total relative influence score 13.49:**

J. Phys.D: Appl. Phys**.** (Srf= 1.81224), Langmuir (Srf= 3.85781), Journal of Nanoparticles Research (Srf= 2.81917), ARKIVOC (Srf= 0.47705), Journal of Polymer Science Part A: Polymer Chemistry (Srf= 2.67278), SYNTHESIS-STUTTGART (Srf= 1.19532), Journal of Polymer Science Part B: Polymer Physics (Srf=2).

3 patent applications were submitted. The results were presented at **59 international scientific meetings**. **The research team members have coordinated 9 national projects and participated**

as partner in 2 international projects (FP6-Nanofun-Poly, 2004-2008 and FP7 MagPro2Life, 2009-2013).

Quality of human resources

The research team consists of 7 researchers and 1 PhD student, having complementary expertises: engineering physics, chemistry, physics. In the framework of a new financed project POS-CCE in 2010, Prof. Jurgen Liebscher from Humboldt University Berlin has joined the team. He is a well known personality in the scientific field of synthesis chemistry with a rich research (232 papers published in journals listed ISI, 169 patents). In the research team have been employed 2 young chemists researchers from abroad, one as post-Doctoral position and the other as PhD student. They are working in the field of synthesis of functionalized hybrid materials for applications in nanomedicine and organocatalysis. **The average age of team personnel is 39 years.** The team members have a high level of specialization and they have performed research stages at prestigious institutions from abroad: *Humboldt University Berlin, Germany*, *Institute of Polymer Science CSIC Madrid, Spain, Institute des Materiaux Jean Rouxel, Nantes, Lund University Sweden.*

Collaborations and partnerships with other prestigious institutions in the country and abroad

National collaborative partnerships: Romanian Academy-Timisoara Branch, National Institute R&D for Materials Physics Bucharest, Babes-Bolyai University Cluj-Napoca.

International partnerships: *Institut fur Chemie, Humboldt University Berlin; Institute of Polymer Science, CSIC Madrid; Institute des Materiaux Jean Rouxel, Nantes; Solae Danemarca, MERCK, ETH Zurich, Elvetia; Karlsruhe Institut für Technologie (KIT), Karlsruhe Germania; Universitätsklinikum Erlangen - Section for Experimental Oncology and Nanomedicine(SEON).*

Quality of infrastructure

Based on the funded research projects the research team contributed to the purchase of new equipments which increased the performances of the research activity: XPS, AFM/STM, SQUID. The POS-CCE project offered the opportunity to create a new chemistry laboratory, well equipped to satisfy the highest requirements of the research work of the team

Future development of the team

The scientific results and know-how accumulated, as well as the existing research infrastructure will stimulate the extension of researches in the field of functionalized hybrid materials based on polymers and magnetic nanoparticles applicative oriented to nanomedicine, biotechnology, new recyclable organic catalysts. New young researchers (PhD students, postDoc) will be attracted into the team activities. Collaboration agreements with institutions from abroad will be developed allowing common research activities with the team and further accessing European funding instruments.

Self-Assessment Report: Team 7 - Spectroscopy of the nanostructured and multifunctional molecular and supramolecular systems

Quality of the research-development activity

Innovative methods:

1. Preparation of multifunctional nanostructured systems by ultra sonication and freeze drying;

2. Physical-chemical characterization of supramolecular assemblies containing bioactive and nanostructured substances by molecular spectroscopy, XRD, XAS and XPS on powder samples;

3. Development of new FTIR and spectrofluorimetric techniques to identify formaldehyde resins;

4. Development of analysis techniques for global radioactivity of mineral waters determination;

5. Design and implementation of the software products for the structural and energetic properties characterization of the nanostructured multifunctional systems.

In the 2007-2011 period: we have coordinated a total number of 13 projects from peer-reviewed competitions (positions CF2, CF3, CF11, CF12, F1, F2, F7, F61, F65, F69, F70, F80 and F86 in the INCDTIM projects list) and four Core National projects, respectively.

Research topics, projects of partnership type:

Encapsulation of bioactive pharmaceutical substances in cyclodextrins and/or chitosan - obtaining, physical-chemical, electronic and structural characterization

Three projects from peer-reviewed competitions: polymorphic forms of drugs and cyclodextrins-drug supramolecular systems (F7); biocomposites with chitosan and porphyrins used in photodynamic therapy of cancers and with hydroxyapathite for endodonthy, respectively (F70, CF11). Supramolecular systems for controlled release of bioactive principles; bioactive substances encapsulated in chitosan for X-ray dosimetry (two CORE supported projects).

Description based on spectroscopic methods of global, local and electronic structure properties of oxidic vitreous, catalytic and photocatalytic systems

Projects from peer-reviewed competitions : vitreous oxide systems based on boron and bismuth with 4f transitional ions (Gd or Eu) (F69); tellurate and germanate vitreous systems with application in telecommunication (F80); oxidic systems with special properties (F86); recovering of the transitional metals from waste catalysts (F65); reduction of the gaseous emissions with green house effect using supported metal catalysts (CF2); supported metal catalysts with direct application in the environment protection (CF3); photocatalytic systems for solar cells (CF12); photoelectrocatalytic systems for hydrogen production (F1). Modelling structural and electronic properties of metallic aggregates with catalytic properties); highly disordered oxide systems-Reverse Monte Carlo modelling (Two CORE supported projects).

Economic demands:

- 2010 beneficiary "VIROMET" Victoria: FTIR and spectrofluorimetric analysis of formaldehyde resins (i); 2010 and 2011 beneficiary: Carpathian Spring S.A: radioactivity analysis of water samples (ii); 2011 beneficiary: INCDO INOE-2000 Branch ICIA Cluj-Napoca, radioactivity analysis of volcanic tuffs (iii).

Valorization of the obtained results in these projects:

In the period 2007-2011 a total number of 59 ISI articles were published; 20 papers have as main author members of the group; citations: 67; SRI=38.6113; non-ISI publications: 9; ISI papers published with foreign authors: 11; non ISI papers published with foreign authors: 8.

Relevant papers for our group (average relative influence score 1.40835) were published in:

Anal. Bioanal. Chem.; J. Incl. Phenom. Macrocycl. Chem.; J. Molec. Struct.; *J.Nanopart. Res.; Superlattices and Microstructures.*

Patent application "Procedure of micro-nanostructuration and self assembling of chitosan and bioactive anti inflammatory drugs"

Editors: C.M. Muntean, and I. Bratu; Editor in chief: A. Hernanz for a review book: "*Insights into DNA structure and dynamics*", Transworld Research Network Publishers, Trivandrum, Kerala, India, 2009, ISBN: 978-81-7895-407-3; author to the chapter "Vibrational relaxation of nucleic acid components", A. Hernanz, I. Bratu, J.M. Gavira

Quality of human resource

The group shall be composed of: -CS I (two), -CSII (one), -CSIII (two), -CS (two), one post doc, one PhD student, one technician.

Dynamics of the human resource: promotion from CSIII to CSII-one; promotion from CS to CSIII-two; promotion from research assistant to CS-two.

Gaining professional skills of young PhD students (two RU-TD CNCSIS projects)

Infrastructure quality

- *FTIR JASCO 6100 spectrometer* with accessories and multiple users, *Able - Jasco FP-6500 spectrofluorimeter,* DSC-*60 Shimadzu differential scanning calorimeter*, *Christ Alpha 1-4 LD freeze drier*. First two equipments correspond to positions IS4 and IS10 in the equipment list.

-Software computer packages used for the global and local structure analysis of the crystalline and amorphous nanostructured systems (developed by the group or purchased)

Future strategy: *Future project proposals:*

Software platform dedicated to the nanostructure analysis of advanced materials, based on powder X-ray diffraction data analysis; nano dimensionality analysis techniques for metallic clusters with catalytic properties.

Investigation by nondestructive *vs* destructive methods of the constituent materials of heritage religious art objects for their conservation, restoration and valorization.

New vitreous materials composed of heavy oxides and based on co doping mechanisms with applications in telecommunications.

Vitreous materials and heavy concrete used as shields for radioprotection.

International Collaborations

1. *International Cooperation between Leiden Institute of Chemistry, The Netherlands and National Institute for R&D of Isotopic and Molecular Technologies Romania.*
2. *Scientific Cooperation Agreement between BEPC National Lab Beijing Peoples Republic of China and National Institute for R&D of Isotopic and Molecular Technologies Romania.*

Team E7:

Name	Research experience abroad	Field of interest (publications/citations-2007-2011)
Dr. Ioan Bratu	UNED Madrid, Spain	Infrared spectroscopy (36/48)
Dr. Nicolae Aldea	IHEP, Beijing Synchrotron, China BESSY Synchrotron , Germany	X-ray absorption spectroscopy, X-ray diffraction (10/17)
Dr. Simina-Virginia Dreve	IIO Groningen - radiochemistry Evaluator and Project Technical Assistant at European Commission	Spectrofluorimetry, radiochemistry, multifunctional chemistry (9/4)
Dr. Irina Kacso	Zinsser Analytique, Frankfurt – high-throughput crystallization	Solid form screening, Thermal analysis (12/11)
Dr. Vasile Rednic	Osnabrück University, Germany IHEP, Beijing Synchrotron, China	Magnetism, X-ray photoelectron spectroscopy (7/2)
Dr. Ing. Ramona - Crina Suciu	-	Materials science and engineering (5/3)
PhD Student Marcela-Corina Rosu	-	Photochemistry of nanostructured materials (5/2)
Tehn. Sorina Ciupe		Solid forms preparation by different methods, infrared spectra measurements

Self-Assessment Report: Team 8 - Numerical Modeling

Human resource: All team members hold PhD in physics, except #9 (BEng)

Nr.	Name	Age	Expertise and fields of research
1.	Tosa Valer	56	Laser-atom and laser-molecule interaction, modeling migration in food contact materials, attosecond XUV generation
2	Munteanu Michaela Cristina	55	Vibrational spectroscopy of nucleic acids; molecular structure and dynamics
3	Morari Cristian	41	DFT simulations of physico-chemical properties of DNA and nanostructured systems; molecular electronics
4	Bilc Daniel	39	Material properties modeling within DFT; thermoelectric, ferroelectric and multiferroic materials; physics of multifunctional materials
5	Bogdan Diana	38	Modeling the interactions of material species on surfaces within DFT; properties of organic molecules adsorbed on surfaces
6	Bende Attila	38	Supramolecular design; electronic excited states; molecular modeling; laser-molecule interaction
7	Buimaga-Iarinca Luiza	30	Statistical modeling in bio-molecular systems; DFT calculations for molecular species adsorbed on metallic surfaces
8	Kovacs Katalin	31	Ultrashort laser pulse interaction with gas media, tracing electron trajectories in laser-atom and laser-molecule interactions
9	Hojbota Calin Ioan	22	programming, develops user interface for the applications, building models for laser-molecule interaction

Research topics and main results:

The modeling duty, as we understand it, is to reveal the physics and/or chemistry behind experimental data which are often difficult to explain. In addition we try to predict new facts and features based on our developed physical or chemical models. Numerical modeling group is mainly focused on investigating the structure of atomic, molecular or bio-molecular systems and describing the interaction processes in which these systems are involved. The results are obtained in collaboration with other teams in our institute (teams7, 9, 10, and 11) or with laboratories abroad. One must outline that *international collaboration* is the specific feature of the team.

Main research directions:

A) *Macroscopic modeling of XUV and soft X-ray production through high-harmonic generation in atomic and molecular gases.* The main goal was to obtain and characterize ultrashort pulses

in the attosecond domain generated in atomic or molecular gas media by two laser pulses of different frequencies or by one laser pulse and a THz radiation. Experimental data were obtained in collaboration with leading groups in the field: Politecnico di Milano, Max Planck Institute for Quantum Optics, Kansas State University, University of Szeged, Korea Advanced Institute for Science and Technology.

B) *Modeling diffusion in multilayer systems.* The long-standing collaboration with a private research company, FABES GmbH Munchen, led to the development of several models describing migration of chemical substances through polymer systems or composites used as food packaging materials. The collaboration goes on within the FP7 project FACET having as main goal the assessment of the European customer exposure to potentially dangerous chemicals coming from flavors, additives and food contact materials. Heat diffusion is also a topic of collaboration with E9 team.

C) *Theoretical study of electronic band structures of one dimensional infinite polymer chains* in case of biomolecules, in collaboration with the Friedrich-Alexander University Erlangen-Nurnberg. The nature of molecular interactions between the DNA and the histone proteins in the nucleosomes at molecular level are investigated, and the influence on cancer initiation is especially envisaged.

D) *Coherent radiation interaction with molecular excited states* and processes followed by these excitations: excited state relaxation, ionization charge transfer, etc. This research is a part of a European FP7 ATLAS project which aims at inducing DNA-protein cross-linking using coherent laser radiation. A direct applied goal in this research is early detection of cancer development.

E) *Study of molecular adsorption on metal surfaces using DFT.* The information produced focus on (i) determining the adsorption geometry on the surface (i.e. the relative position of molecules on the surface, and intrinsic molecular structure changes induced by adsorption, respectively) (ii) determining the adsorption energy (iii) elucidate the mechanisms of interaction that occur at the molecule-metal interface. As systems of interest we use DNA fragments (i.e. DNA bases, nucleosides and base pairs). We focus on the development of methods and computational techniques that allow modeling the effects of surface defects on the vibration modes of adsorbates.

F) DNA structural changes and dynamics. Main topics are: a) elucidation of the nature of the changes in DNA structure, caused the interplay between physical-chemical parameters; b) establish the (sub)picosecond dynamics in nucleic acids and their constituents; c) ultrasensitive detection of DNA using surface-enhanced Raman spectroscopy (SERS).

Scientometric data: ISI papers 2007-2011: 70 of which 41 worked out in international collaborations. The relative article influence score of 38 articles is > 0.3, while for 12 articles it is >

1. We succeeded publishing in top physics/chemistry journals like: ACS Nano, Phys. Rev. A, Phys. Rev. B, J. Phys. B, Opt. Lett., Opt Express, J. Chem. Phys., J. Organic Chem.

Communications to international conferences: 62

Projects financed: In the period analyzed the team won seven projects in national competitions, four of them being under development. Our team participates in two FP7 projects which will end in 2012. In the most recent PNII call we won one PD (postdoc) and two TE (young team) projects.

New directions of research

By the end of next year the research infrastructure of our Department will be heavily renovated. The members of the team will be actively involved in collaborating on new topics of experimental research stimulated by the new instruments available. In addition we develop new directions of modeling:

- *Characterizing highly excited states in complex molecules as a result of their interaction with an ultrashort laser pulse*. Using methods of computational chemistry we will investigate the excitation and relaxation paths of various molecular systems in interaction with a strong pulsed UV radiation (PNII TE project)
- *Using combined ultrashort laser pulses and THz radiation to generate single attosecond pulses.* A numerical model will be extended to model macroscopic high order harmonic generation in two fields of incommensurate frequencies (PNII PD project).
- *First-principles modeling of $SrTiO_3$ based materials for thermoelectric applications.* The study and optimization of the thermoelectric (TE) properties of promising oxide materials for high temperature TE applications (heavily-doped $SrTiO_3$, and Sr-based $AO[ABO_3]_m$ naturally-ordered materials) by performing electronic and transport calculations (PNII TE project)
- *Applications of organometallic compounds in nanotechnology (molecular electronics)* is a newly initiated direction. Our target-systems are organometallic systems (i.e. metallocene molecules).

Infrastructure

a) **Linux Cluster** with 2 x AMD Opteron 275 – workstation (4 nodes 8 GB RAM); 1 x AMD Opteron 2224 SE – workstation (4 nodes, 16 GB RAM); 3 x Intel E5430 – workstation (8 nodes, 16 GB RAM)

b) **Linux Blade System** with 16x Intel Blade (16 nodes, 16 GB RAM);

Access to Computer Center of Catholic University of Louvain-la-Neuve

Existing software: **Gaussian 03** and **Molpro 2010.1** for MCSCF, MRCI, CASPT2 and non-adiabatic coupling matrix elements; **CPMD** for non-adiabatic molecular dynamics; nonadiabatic 3D model for ultrashort pulse propagation and high-harmonic generation; numerical model for migration in multilayer polymer systems.

Self-Assessment Report: Team 9 - PHOTOTHERMAL AND MICROWAVES APPLIED RESEARCH

Quality of human resource. The team is composed by 1 CS I (**D. Dadarlat -** photothermal phenomena, detection and emission of radiation, critical phenomena and phase transitions, magnetism); 2 CS II (**E. Surducan** – microwave circuits design, material characterization and processing by microwaves methods and **C. Neamtu** - crystal grow techniques, calorimetric characterization); 1 IT I (**V. Surducan** - electronic design and prototyping (RF, MW), microcontroller development applications); 1CS III (**M. Streza** - photothermal phenomena, thermography); 3 CS PhD students (**I. Lung** - chemical analysis and chromatographic methods, microwave –plant system interactions characterizations, **M. N. Pop** - photothermal phenomena, IT, electronics and **C. Tudoran** - RF /MW plasma generators and applications.

Some of the members of the team participated to working stages in well known foreign laboratories as follows: **D. Dadarlat:** Lebedev Inst. of Physics, Moscow, Rusia; **"**Tor Vergata" University Rome, Italy; Agricultural University Wageningen, Holland, University of Reims and Dunkerque, France; University of Campinas, Brasil; **C.Neamtu -"**Tor Vergata" University Rome, Italy; Agricultural University Wageningen, Holland; **M. Streza - "**Tor Vergata" University Rome, Universite du Littoral Dunkerque, France; Universite Paris VI, France (present); **E. Surducan, V. Surducan –** Sandbridge Technologies Inc., White Plains, NY, USA; **C.Tudoran** - University College Dublin, Ireland.

Quality of the research activity.

Number of published papers in ISI journals: 34; total relative influence score: 27.329

Number of published papers in non-ISI journals: 21

Number of papers published in cooperation with other universities: 8

Number of citation of the team (2007-2011): 87

Book chapters: 2 (Kerala and InTech, Eds.), in cooperation with other universities: 1

Patents: - international: 2 (US 7,746,276 / 29 Jun.2010 and EU 1854169/ 14.11.2007) + 1 pending (KR 20070102491 (A) /18.10.2007); - **national**: 3: (RO-112063/2008, RO-00122152/2009, RO-A/00833–06.12.2007–BOPI nr.3/146 / 30.12.2010)

Medals obtained at national and international exhibitions of patents: 5

Participation at international conferences: 28 conferences/ 48 (7 invited) papers

Participation at international exhibitions of patents: 3 exhibitions/12 exponents

International cooperation with: Tor Vergata University Rome, Italy; Universite du Littoral, Dunkerque, France; University College Dublin, Ireland; Tampere University of Technology, Finland; University of Victoria, Canada; Institute de Physique du Globe de Paris, France.

Activity of referee: D. Dadarlat: J. Food Engn., Meas. Sci. Technol, Int.J. Thermophysics, J. Phys. D- Appl. Phys., Instr. Sci. Techn., Food Biophysics, J. Physics: CS, Appl. Phys. A, Central

European J. Phys., Int. J. Mol. Sci., J. Mat. Sci., Thermochimica Acta, Int. J. Thermal Sci.; **E. Surducan:** J. Dig. Multimedia Broadcasting, Int. J. of Phys. Sci, Bioelectromagnetics.

Research projects coordinated by the team members (2007-2011):

1. National: 5: Project CEEX-Agral 65/2006- 2008; Project CEEX 05-D11-80/2005-2008; Project CEEX 06-11-38/2006-2008; PNII Nr.51-098 /2007-2010; CAPACITIES Module I – Large investment project Nr. 2 PM/I/2008-2012.

2. Bilateral (international): 2: Bilateral project Romania (INCDTIM Cluj) – Italy (Tor Vergata University Rome); Brancusi Project 204/2009 between INCDTIM Cluj and Universite du Littoral Dunkerque France.

3. Active projects: 1: PN II –ID-PCE-2011-3-0036

Technological assistance to: "ISDC Integrated Systems Development Corporation", SC.TRAECT SRL, Dir. Radiocomunications Cluj.

Topic of research

Contact and non-contact photothermal techniques (period 2007-2011)

1. *Photopyroelectric calorimetry and spectroscopy and applications*: (i) development of theoretical aspects and particular detection cases; (ii) design of various experimental set-ups; (iii) applications: investigation of quality of various foodstuffs; detection of molecular associations in binary and isotopic mixtures; thermal characterization of composite materials, liquid crystals and ferroelectric materials; detection of phase transitions; PPE spectroscopy of solids.

2. *Combined contact-noncontact photothermal calorimetry (started in 2010)*: (i) development of theoretical aspects and particular detection cases; (ii) design of various experimental set-ups; (iii) applications: thermal characterization of composite materials.

Microwave processing and characterization of materials (period 2007-2011)

1. *Development of microwaves methods for thermal processing, dielectric and magnetic characterization of composite materials;*

2. *Thermal and non-thermal processing of materials by microwaves power – including microwaves /RF plasma;*

3. *Design and prototyping of microwaves equipments for microwaves high and low power applications*: transducers, control embedded systems, microstrip circuits, specific applicators/antennas;

4. *Microwaves interactions with biological systems*: environmental microwaves power distribution measurements, effects of the microwaves on plat grow, medical applications;

Available equipment of the team: radiation sources: lasers (HeNe, YAG, diode laser); lock-in selective nanovoltmeters (SR 830); thermostatic bath; multimeters (6 and 8 digits); programmable

power supply; detectors of radiation; Q150R ES deposition system; optomecanics; microwaves power-meter Agilent N1911A 50MHz-50GHz; vector network nnalyzer (VNA) Agilent PNA-L, N5230A 10MHz-40Ghz; spectrum analyzor Agilent PSA E4448A 10MHz-325GHz; microwaves analog signal generator Agilent PSG E8257D DC-325 GHz; LPKF / Essemtec multi-layer (4-8 layers) professional PCB prototyping line; SDTQ-600 simultaneous thermo gravimetric and differential calorimetry DSC-TGA heat flow analyzer; microwave synthesis owen; microwave sample preparation platform system SYNTHOS 3000- Anton Paar; computers, printers, scanners, etc

Future development

Topics of research: Photothermal: (i) High accuracy photothermal calorimetry for magnetic nanofluids; (ii) Combined PPE-PTR calorimetry for investigating thermal properties of composite materials; (iii) Photothermal radiometry. **Microwaves:** (i) Basic research regarding microwaves interaction with biological complex systems at high frequencies (50GHz-325GHz), microwaves circuit design and signal detection by radiometric effects; (ii) Applications of the microwaves effect interactions (thermal processing, plasma induced), ionized gases characterization by microwaves method, transducers by microwaves emission/reception (humidity, conductive material granulometry, temperature measurements, etc.)

Activities to support the future development:

- 2 international cooperation projects with (i) Universite du Littoral, Dunkerque and (ii) Institute de Physique du Globe de Paris, France were already proposed and one of them (ii) was selected ;
- acquisition of equipment: an IR camera (to be bought) and a measurement system of dielectric and absorption effect in the microwave range DC-325GHz (system recently acquired) on project Nr. 2 PM/I/2008-2012
- one of the members of the team (MS) is presently working (post doc grant) at Universite Paris VI in the field of radiometry/thermography;
- one of the members of the team (MNP) will participate (Feb-Apr 2012) to a training at Universite du Littoral Dunkerque in the field of PPE and PTR calorimetry.
- two members of the team (ES, VS) will participate (Nov.2011) to a workshop at Institute de Physique du Globe de Paris, France, in the field of convection experiments with microwaves heating;
- two PhD students (IL and CT) of the team are involved in research of RF plasma and related applications in studies of microwaves effect on plant growing.

Self-Assessment Report: Team 10 - Structural Analysis in Solids

Human resources:

Name	Research experience abroad	Field of interest / publications*
Dr. Filip Claudiu	MIT Cambridge / Max Planck Institute for Polymer Research Mainz / RWTH Aachen	Solid-state (SS) NMR spectroscopy: methods developement and applications 36 articles (over 400 citations)
Dr. Borodi Gheorghe	BESSY Berlin / University of Amsterdam	Powder and single crystals X ray diffraction; 70 articles (over 150 citations);
Dr. Filip Xenia	Ruhr University, Bochum	Molecular modeling on solids / SS-NMR spectroscopy; 26 articles (over 100 citations);
Dr. Tripon Carmen	Warwick University	SS-NMR spectroscopy; 11 articles
Dr. Pop Mihaela **	Avantium Ltd. Amsterdam	Solid forms screening; 15 articles; 6 pattents
Dr. Grosu Ioana / (Postdoc)**	Leipzig University	Coordinative compounds; Supramolecular chemistry; 3 articles
Martin Flavia / (PhD student)**	Institut de Recherche en Chimie Organique Fine, Rouen	Supramolecular chemistry; 4 articles
Miclaus Maria / (PhD student)**		Powder X ray diffraction;
Muresan-Pop Marieta (PhD student)**	University of Bologna	Single crysal growing; 2 articles

*Only regular articles in ISI ranked journals; **Have joined the team in 2010 and 2011 as a consequence of extending our area of research

Research activity in the last 4 years:

Research topics and the main results:

Solid-state (SS) NMR methodological developments (new theoretical tools/models and experimental schemes):

Elaboration of a new symbolic computation tool named SD-CAS (Spin-Dynamics by Computer-Algebra-System) for describing the Liouville-space quantum evolution in systems of arbitrarily large nuclear spins: theoretical foundation and proof-of-concept by its practical implementation for systems of identical ½-spins

Improved experimental schemes and theoretical models to increase the accuracy with which ^{1}H-^{1}H distances can be extracted from two-dimensional (2D) correlation spectra obtained by employing the CHHC and ^{1}H-^{1}H Double Quantum (DQ) solid state NMR techniques – collaborative works with the SS-NMR Group (Warwick University – Prof. Steven P. Brown), and MIT (Prof. Robert G. Griffin)

Applications of X-Ray diffraction:

Structural investigations on a wide range of organic and inorganic materials: inclusion compounds of cyclodextrin, active pharmaceutical ingredients (API), polymers, intermetallic compounds, and glasses – mainly through collaborative works with other research groups

Modern approaches for new solid forms screening of APIs and structural characterization on powders – this is the major event in the dynamics of our research group, which represents an extension of its activity towards pharmaceutical applications:

Implementation at our institute of advanced *high-throughput* technology for producing and characterizing new solid forms (polymorphs, co-crystals, solvates, hydrates, salts) of APIs. This is carried out through an EU funded project, and had brought so far the following benefits: (i) an infrastructure unique in our country for systematic solid state characterization of pharmaceutical compounds has been created, (ii) multidisciplinary was strengthened by attracting new members with expertise in solid forms screening and supramolecular chemistry, which is beneficial for the future evolution of our research team.

Developement of multi-technique approaches that combine X-Ray powder diffraction (XRPD) with suitably designed SS-NMR techniques and *in silico* methods for crystal structure determination on microcrystalline powders. They are important for the pharmaceutical industry, when single crystals of sufficient size and quality cannot be grown.

Articles in ISI ranked journals:

In the period 2007-2011: a total 34 articles, out of which: 9 articles as main authors, and 25 as co-authors. The latter have resulted from collaborations with research groups from abroad (10), and from the country (15). The most relevant journals in which we have published are *PCCP, Acta Crystallographica B, J. Magnetic Resonance* (as main authors), and *Spectrochimica Acta A, J. Inclusion Phenomena and Macrocyclic Chemistry, J. Non-Crystalline Solids, J. Alloys and Compounds* as co-authors, all with relative influence scores close to-, or greater than 2. The

cumulated relative influence scores for all the publications is 43.7 (that is, an average of ~ 1.3 / article).

The most important scientific meetings attended:

European Magnetic Resonance Conference (EUROMAR) in 2007 (Tarragona, Spain), and 2008 (Sankt Petersburg, Russia)

Experimental Nuclear Magnetic Resonance Conference (ENC) in 2007 (Daytona Beach, USA)

Coordinated projects:

In the period 2007-2011: we have been coordinated a total number of 5 projects from peer-reviewed competitions, out of which four are financed through national research programs, and one from EU Structural Funds (position CF20, CF38, CF40, F15, and F83 in the INCDTIM projects list).

Available infrastructure:

Bruker Avance D8 powder diffractometer, *Oxford Diffraction Supernova* single crystal diffractometer, *Bruker Avance III* 500 MHz solid-state NMR spectrometer equipped with a full range of probeheads (including ultra-fast MAS probe), state-of-the art solid forms screening laboratory (main equipment: *Zinsser Crissy XL* parallel crystallization platform, *Eyala* benchtop organic synthesizer, *pION μDISS* dissolution rate profiler, *Buchi P12 EasyVac* multivapor). They correspond to position IS 30, 31, 37, 38, and 39 in the equipment list of INCDTIM.

Perspectives for future developments:

Gain the capability and expertise to routinely: (i) carry out systematic solid form screening of APIs by *high-throughput* crystallization technologies, and (ii) perform structural characterization on powders by employing alternative multi-technique approaches applicable when the new solid forms cannot be grown as single crystals. We plan to exploit the experience accumulated at the end of the EU funded project to make the transition from the present research, mostly of academic interest, to applicative research offered primarily to pharmaceutical companies.

Exploit the newly installed solid-state NMR infrastructure to: (i) increase the scientific productivity of our team – so far, our solid-sate NMR experimental work have been performed through collaboration with other research groups, (ii) diversify the area of current solid-state NMR applications (according to the recently submitted project proposals, the following topics will be considered: study of micro/nanogels as drug delivery vehicles, and study of fibrous protein based biomaterials).

Self-Assessment Report: Team 11 - Self-Assembled Molecular and Biomolecular Systems

Contact: Dr. Ioan Turcu**; Research team**: Dr. Ioan Turcu, Dr. Mircea Bogdan, Dr. Radu Brătfălean, Dr. Silvia Neamtu, Dr. Calin G. Floare, Dr. Adrian Pirnau, Dr. Nicoleta Tosa, Dr. Mihaela Mic, Dr. Adrian Calborean, Phys. Bogdan Cozar, Tech. Carmen Bugeac.

Research topics:

- Intra- and inter-molecular interactions, protein – ligand interactions;
- Cyclodextrins inclusion complexes with biomolecules of pharmaceutical interest;
- Molecular recognition and self-assembling processes;
- Self-assembled molecular structures (monomolecular layers, molecular nano-capsules);
- Fabrication and characterization of supramolecular structures with controlled architecture.

Main research results:

- *Scientific papers in ISI ranked journals:* 32, with a cumulated "**R**elative **I**nfluence **S**core" (RIS): 28.49, of which 14 have a RIS> 1, 12 have a 1 > RIS> 0.3 and 6 have a RIS <0.3. Eleven of these papers have a team member as lead author and for the other 21 papers team members are co-authors. Seven of the coauthored publications were developed with foreign partners.
- *Scientific papers indexed in international databases:* 12;
- *Participation at 80 international scientific conferences;*
- *A book chapter in Progress in Optics Research*, ed. Maximilian N. Schulz, *Nova Science Publishers, Inc. New York.*

The journals where the main papers have been published are: Journal of Biomedical Optics (RIS = 2.5803), Journal of Organic Chemistry (RIS = 2.000), Journal of Optics A: Pure and Applied Optics (RIS = 1.8174), European Journal of Medicinal Chemistry (RIS = 1.738), International J. of Molecular Sciences (RIS = 1.5719), J. Physical Chemistry A (RIS = 1.5009), Supramolecular Chemistry (RIS = 1.258), Vibrational Spectroscopy (RIS = 1.274), Journal of Pharmaceutical and Biomedical Analysis (RIS = 1.238), Magnetic Resonance in Chemistry (RIS = 1.090)

- *Applications for national patents:* 1;
- *Public national and international funds:* Team members participated in the last four years as Director / Coordinator of the project in 11 national research projects which were granted on a competitive basis. Team members are also involved in research on two European FP 7 projects.
- ***Major ongoing projects**:* „Bioligand - macromolecule intermolecular interactions as probed by spectroscopic and microcalorimetric techniques" - project worth about 1.5 million lei, won in the 2011 Ideas Programme competition and "Modernization of Molecular and Biomolecular

Physics Department", project worth about 30 million lei, won in the 2008 competition of the Infrastructure Modernization Programme, which benefits of substantial funding for the 2011-2012 period.

Human resource quality

The degree of specialization: The team includes 10 researchers, 9 of them having PhD in physics or chemistry, and the youngest team member is a doctoral student which will defend his thesis in December, this year. According to their scientific degrees we have two Scientific Researchers I, a Scientific Researcher II and 7 Scientific Researchers III. In addition to the 10 researchers the team benefits also from the contribution of a certified technician. The age-distribution is well balanced. Beside the experienced researchers which are over 40 years old (64, 56, 54, 44, 44) we have the young component of the team (38, 35, 32, 30, 29) which assures a staff average age of 42.6. The research team is highly qualified, an important number of its researchers benefiting from various research stages at universities and / or renowned research institutes. In this respect we mention three examples: Dr. Radu Bratfalean with a doctorate at the University of Oxford, UK and postdoctoral research fellowships at the University of Southampton, UK Dr. Nicoleta Tosa, postdoctoral research fellowships at the University "Joseph Fourier", Grenoble, France, and Dr. Adrian Calborean, with a doctorate at Commissariat à l'Energie Atomique, Grenoble, France and postdoctoral fellowships at École Nationale Supérieure de Chimie de Paris, France. In all cases, the modern research topics addressed by the team and the massive modernization of the research infrastructure from recent years have been compelling arguments for their reintegration in research in Romania.

Collaborations and partnerships with other high-prestige institutions from home and abroad

Partnerships with Romanian institutions: "Babes-Bolyai" University, Cluj-Napoca, Faculty of Physics and, respectively, Chemistry; University of Medicine and Pharmacy "Iuliu Hatieganu", Cluj-Napoca; University of Medicine and Pharmacy "Carol Davila", Bucharest; University "A.I. Cuza", Iasi; University of Agricultural Sciences and Veterinary Medicine, Cluj-Napoca; Cluj-Napoca Technical University; National Institute for Research and Development for Physics and Nuclear Engineering "Horia Hulubei", Bucharest; National Institute for Research and Development for Cryogenic and Isotopic Technologies, Ramnicu Valcea.

International partnerships:

Ongoing: University of Cape Town, South Africa;

Future: 1) Syracuse Biomaterials Institute, Syracuse University, NY USA, 2) University of Wisconsin-Milwaukee, USA, 3) Commissariat à l'Energie Atomique, Grenoble, France.

The quality of the infrastructure (main equipment)

1) NMR spectrometer BRUKER Avance III 500 UltraShield,; 2) Clean room for the development of molecular technologies; 3) Integrated equipment for "molecular ink printing" (DipPen Nanolithography); 4) NTEGRA AURA platform (NT-MDT) for atomic force microscopy with integrated Tip Enhanced Raman Spectrometer; 5) Nano ITC 2G isothermal titration calorimeter ; 6) UV-VIS Jasco V-550 Spectrometer; 7) High power microwave field installation for sample treatment; 8) Automated inverted microscope. With the exception of the equipment at position 6 all the other was purchased in the last four years, most of it being acquired in this year on the Research Infrastructure Modernization project, mentioned above.

Perspectives of development: Next year the research and technological development infrastructure will benefit from the acquisition of a coupled MBE-STM system (Molecular Beam Epitaxy – Scanning Tuneling Microscopy), a nanoimprinting fabrication system and a vibrational circular dichroism spectrometer. A concern of permanent interest will be the rejuvenation and the specialization of personnel offering graduate, doctoral and young researchers top conditions for a specialist training of ultra high level.

The research topic in the coming years will focus on *technological development component* with an emphasis on *developing the team's expertise in the field of molecular technology*. We envisage the development of very small scale molecular systems, based on advanced molecular technologies, to be applied in high technology areas: *molecular electronics, high-selectivity high-performance sensors based on molecular recognition processes, self-structured molecular systems with controlled architecture and functionality, intelligent molecular materials.*

We also aim to *increase the international visibility and attractiveness* of our research group so to be included in R&D consortia with international participation. In this respect we will initiate close collaborations with research groups with a close profile, mainly from European countries. All our proposals in preparation provide for the necessary funds for training stages of our members in high performance research centers from abroad.

We believe that by the end of next year our research infrastructure will be relatively complete and highly competitive. The main concerns of the coming years will focus on a substantial increase of staff competence, attracting funds through a large number of proposals to be submitted to competition based funding programmes, and the development of a sustained activity of research and technological development in the domain of molecular supramolecular and biomolecular sciences and technologies.

Self-Assessment Report: Team 12 – Isotopic technologies and labeled compounds

The team

The team is composed of 14 pearsons: Eng. Mihai Gligan IDT I, Dr. Ing. Kaucsar Martin CS I, Dr. chem. Damian Axente CS I, Dr. Chem. Simion Dronca CS II, Dr. chem. Camellia Grosan CS III, Drd. Chem. Codruta Varodi CS, Drd. Chem. Ancuta Bala CS, PhD Chem. Cristina Marcu CS, PhD. Chem. Adriana Vulcu CS, Ing. Chem. Virgil Stoia CS, Ligia Pop techn., Simion Albu techn., Vasile Oarga techn., Ioan Corojan techn. The team is supported by two consultants, specialists in isotope separation, who contributed to the team results and can further contribute to the development of research projects: Dr. chem. Aurel Baldea CS I and Dr. phys. Ilie Hodor CS I. Group Coordinator**:** Eng. Mihai Gligan, Senior research engineer.

Research topics and results

The team's work is focused on developing technologies in the field of isotope separation, production of isotopes and labeled compounds. The activities, that are mainly technological, were materialized both through research, caried out on 6 projects and by the producing labeled compounds for Romanian and international markets.

The completed projects were fucused on:

♦ Development of technologies for separating of the ^{13}C isotope - 3 projects, resulting in:

- Developing technology ^{13}C separation by cryogenic distillation of CO

- Design and construction of the automated control of the process, computer driven, for the ^{13}C isotope separation by cryogenic distillation of CO;

- Design and construction of an experimental plant and gathering technological data for the separation of $1^{13}C$ through chemical exchange CO_2 - carbamate.

The results obtained so far allow us to get in a final phase of research: design and building of a multiple columns separation plant, cascaded horizontally and obtaining the necessary design data for technology transfer.

♦ Synthesis and production of ^{15}N labeled compounds - 3 projects resulting in:

- Data on nutrient accumulation in plants in various stages of growth and evaluation of fertilizers effects in agriculture

- Development of amino acids and proteins labeled with isotopes by molecular biotechnologies

- Isotope labeled amino acids synthesis and functionalization of nanoparticles of colloidal gold - in progress

The research conducted over the past 4 years was materialized in:

- 18 ISI scientific papers, 10 of the having a total impact factor of 8.634 and a relative influence score of 6.059

- 48 papers at national and international conferences, 42 of them being international conferences. Besides research results exploited by scientific papers published or presented at conferences, the team's research have produced:
- 2 experimental plants and 2 isotope separation and labeling technologies, 1 product of isotopic separation, 3 experimental models for studies of separation, 2 technological studies on isotopic processes, 2 complex technical projects for isotope separation plants and synthesis of labeled compounds, 6 isotopic labeling methods of organic molecules, 2 molecular biotechnologies, 15 organic and inorganic isotopic labeled products delivered to customers.
- 2 patent applications for components of the experimental plant of separation of ^{13}C by cryogenic distillation carbon monoxide

Research carried out has created the possibility of participation in an FP7 project: Asgard - Advanced fuels for Generation IV Reactors, Reprocessing and Dissolution, that started in 2011, in which our team will conduct the research on technology production ^{15}N through isotope exchange in Nitrox system, without waste of sulfuric acid.

Infrastructure

The team has a pretty good infrastructure, materialized by:
- Production plant ^{15}N, experimental plants cryogenic for the separation of ^{13}C through distillation and chemical exchange - designed and built in INCDTIM, and hosted in the buildings that have all the facilities for production or research (currently under renovation and interior decoration)
- Equipment and installations for synthesis and production of labeled compounds - designed on the basis of own technologies. The usage is limited to isotope conversions necessary to produce the labeled compounds required for our customers, for our own research projects or for the research partners;
- Equipments for laboratory and for measurement, analysis and control, acquired over the past five years - gas chromatograph, potentiostat, UV VIS spectrophotometer.
- Liquid nitrogen production plant - which serves our own research and delivers the entire quantity of liquid nitrogen required in INCDTIM, which means about 200 liters of liquid N_2 per week.

Management

Team management is provided by a group consisting of the team leader and the project managers. The management of the team's projects is supported by a person who deals specifically with issues such as equipments and consumables supply, project or reporting forms and the current bureaucratic activity. The staff team is paid according to the budget of their own projects and of those where we are partners and to the scientific performances.

Team Development Plan

From a strategic perspective, the team aims to fully exploit the niche research topics (having an important tradition and being unique at national and even European level) in which we have expertise, to finalize and apply the technologies for ^{13}C and ^{15}N isotope separation and to diversify the area of research to the separation of other stable isotopes of interest: ^{18}O, ^{43}Ca, ^{25}Mg, etc.. The team will specialize in the development of special isotope-labeled compounds in order to meet the requirements of other research teams from INCDTIM or other research institutes and universities, in joint projects. Working with teams participating in the Center for stable isotopes of INCDTIM is an essential direction for the future activity.

Future prospects of the team in the ^{13}C isotope separation enrichment domain are the advanced ^{13}C enrichment using a combination of the two technologies we are working on, and technology transfer. The production of isotopes and labeled compound can be taken over by a spin-off or by industry.

On the other hand, a valorization (not only possible but probable) for the ^{13}C isotope separation technology through chemical exchange CO_2 - carbamate is using this method for the depletion of the $^{14}CO_2$ waste. The radioactive waste comes either from companies that produce radio-isotopes or from nuclear reactors moderated with graphite that are to be soon shut down in EU countries (e.g. England). The problem is very important both environmentally and economically, and creates the possibility of collaboration with industry in developing and scaling the technology that INCDTIM is working on. The team, under the direct coordination of the INCDTIM director, is negotiating with a private company in the UK interested in the technology of carbon isotope separation by chemical exchange CO_2 – carbamate.

The team will also continue the research to improving the efficiency of producing ^{15}N needed for the nitrite type nuclear fuel and will be involved in European projects on this subject.

The team applied, on the last national call, for 5 research projects on isotope separation technologies and labeled compounds.

In order to develop the research directions and projects we are proposing, employing of young specialists in mechanical engineering, chemical synthesis and physical-chemistry of isotopes is a must. The strengthening of the technicians' team, diminished in number through retirement, is also needed.

Self-Assessment Report: Team 13 - Processes with deuterium, catalysis, and nanostructured sensors

Group Coordinator: Dr. Eng. Valer Almăşan, Senior Researcher I

Team members: Dr. Stela Pruneanu, Senior researcher II; Dr. Liliana Olenic, Senior researcher II; Dr. Mihaela Diana Lazăr, Senior researcher II; Dr. Florina Pogăcean, Senior researcher III; Eng. Maria Miheț (PhD student), Senior researcher; Eng. Monica Dan (PhD student), Senior researcher tehn. Ioan Mărginean; tehn. Ioan Ielciu.

Between 2007-2011 the research activity of the team was focused on four main research directions:

- Hydrogen production by catalytic reforming of hydrocarbons and alcohols;
- Applications of H/D isotopic exchange for the synthesis of deuterium labeled compounds and for catalysts reactivity studies;
- Hybrid nanostructures based on metallic nanoparticles and biomolecules/graphenes;
- Catalytic reactions for pollution control processes: denoxification and delignification.

Quality of the research activity between 2007 and 2011.

a.) Publications. A number of 36 papers were published between 2007 and 2011, from which 31 in ISI ranked journals, with impact factors ranging up to *9.95308*. The average relative influence score/ISI ranked paper is of 1.587, while the average number of citations/paper is of 2.686. Other 2 articles are accepted, while another one is under review.

Table. 1. Publications and conferences as results of the research activity (2007-2011).

	Articles				**Books/Book chapters**		**Conferences**	
	ISI	Non-ISI	Internat. Collaboration	Citations	Nat. Publisher	Internat. Publisher	Nat.	Internat.
	31	5	16	94	2	2	4	46
TOTAL	**36 /** *47.60374*[1]				**4**		**50**	

[1]*Relative influence score for the ISI ranked journals.*

b.) Patents and methods.

During 2007 and 2011 the members of the research team were authors/coauthors of 4 patent applications, from which 2 were already granted. Moreover, 4 preparation methods for different nanomaterials were developed. The prepared nanomaterials are based on metallic nanoparticles and aminoacids, DNA, or proteins, and have applications in microelectronics and medicine.

c.) Projects. At present, the research team has 3 projects under development with a total value of ~1.525.800 lei (value for INCDTIM), one as project coordinator, and the other two as partners.

During 2007 and 2011 the members of the group were part of the research teams of other 10 national projects developed in INCDTIM, besides those coordinated by them.

Table 2. The number and the value of the projects coordinated by the members of the research team between 2007 and 2011 (finalized projects or under development).

	National Projects		**International Projects**
Involvement of INCDTIM	Coordinator	Partner	Partner
No. of projects	3	3	2
Value of the projects[1] (lei)	~3.410.000	416.171	~25.800
TOTAL	8 projects / ~3.851.971 lei		

[1]*Value for INCDTIM from the total value of the projects.*

The quality of the human resources is evidenced by the quality of the research activity, as well as by the facts presented below.

The research team is formed of 7 researchers with complementary education and training (chemistry, physics, chemical engineering, biochemical engineering) and 2 technicians. The research team is a relatively young one, with an average age of 43 years, and consists of 5 PhDs and 2 PhD students. The distribution on scientific positions is as follows: 1 senior scientist I (CS I), 3 senior scientists II (CS II), 1 senior scientist III (CS III), and 2 senior scientists (CS).

The fields of expertise of the research group members cover the following:

- Preparation of nanostructured materials based on supported or unsupported metallic nanoparticles, using the following methods: impregnation, deposition-precipitation, sol-gel;
- Characterization of nanostructured materials by: BET, GC-MS, TPD, TPO, TPR, TPRea, UV-VIS, cyclic voltammetry, AFM, TEM, H/D isotopic exchange, etc.

The high level of qualification and excellence of the group are also evidenced by the fact that the majority of the team members have benefitted from one or more scholarships or research internships abroad, in prestigious institutions. Moreover, some of the research team members have refereed for prestigious journals, or were involved in the evaluation process for national/international projects.

Name	**Research experience abroad / Reviewer / Evaluator**
Dr. Eng. Valer Almăşan	♦ Research experience abroad: Institute de Chimie Physique de L'Ecole Politehnique Federale de Lausanne, Switzerland (1974-1975, 1990-1991) ♦ Evaluator in national programs: PN II, CEEX, POS-CCE, Bilateral Agreement IFA-CEA
Dr. Stela Pruneanu	♦ Research experience abroad: Institut für Festkörperphysik, Graz, Austria (feb., oct. 1995), Eotvos-Lorand University, Budapest, Hungary (apr. – june 1997), Teesside University, Great Britain (2004-2006), Newcastle University, Great Britain (2006-2008). ♦ Reviewer: *Electrochimica Acta, Sensor, ACS Nano, J Mater Sci, Langmuir, Particulate Sci Tech*

	♦ Evaluator for *l'Agence Nationale de la Recherche,* France
Dr. Liliana Olenic	♦ Reviewer: *Analyst, ChemComm, African Journal of Food Science*
Dr. Diana Lazăr	♦ Research experience abroad: Iowa State University**,** Ames, USA (2003-2004) ♦ Reviewer: *Reac. Kinet. Mech. Cat.*
Dr. Florina Pogăcean	Research experience abroad: Frederico II Faculty, Napoli, Italy (july-dec. 2005), Faculty of Chemistry, Wroclaw, Poland (febr.-apr. 2006)
Eng. Maria Miheț (PhD student)	♦ Research experience abroad: Helmholtz Zentrum für Umweltforschung - UFZ, Leipzig-Halle, GmbH, Germany (oct. 2003-apr. 2004)
Eng. Monica Dan (PhD student)	♦ Research experience abroad: Universiteit Gent, *Belgium* (2001-2004)

Quality of the infrastructure. The following equipments are exploited by the team members, for the use of the team, as well as for the use of other research groups:

- Sorptomatic 1990, ThermoElectron – Equipment for the determination of specific surface areas (metallic and total) and of the porosity of solid materials (level of exploitation 75%);
- QMS Prisma Plus, Pfeiffer Vacuum – Quadrupole Mass Spectrometer, with gas inlet system (level of exploitation 75%);
- Microactivity Test Reactor, PID Eng&Tech – catalytic reactor with mass flow and temperature control (level of exploitation 75%);
- HG 2200, Claind – Electrocatalytic H_2/D_2 generator (level of exploitation 50%).

Perspectives. The present research group aims the development of the following research topics, which also constitute grant applications:

- New technologies for the production of deuterium labeled compounds for the development of the solid surface structure determination method small angle neutron scattering (SANS);
- Application of H/D isotopic exchange reaction for the determination of the reactivity of metal/oxide catalytic surfaces;
- Advanced nanostructured catalysts for energetic hydrogen production, by reforming of biomass wastes (ethanol, glycerol, etc);
- Advanced denoxification catalysts with low content of noble metals for environmental applications;
- Nanostructured selective catalysts for the production of carbon nanostructures (nanotubes, graphenes);
- Nanostructured sensors based on graphenes and metallic nanoparticles for the detection of pharmaceutical pollutants and for their degradation by amperometric methods;
- Hybrid nanostructures based on metallic nanoparticles coupled with organic molecules with applications in medicine (antiageing, anticancer).

2.3. Representative project

Advanced polymer based nanocomposites with tailored properties and controlled functionality, having great potential for applicability, is a highlight topic research area under continuous development in INCDTIM since 2001. This topic is closely related to the European Research Thematic Area FP7-NMP: Nanosciences and Nanotechnologies, Materials and new Production Technologies.

One of the research groups from INCDTIM Cluj-Napoca obtained valuable results in the field of conducting polymers, being among the initiators of this field of research in our country since 1987. Based on the accumulated experience concerning the properties and applications of conducting polymers, during the last years a dynamic development of the research in the field of advanced polymer based nanocomposites took place in INCDTIM. A multidisciplinary approach has been dedicated to design, preparation, characterization and assessment of applications of polymer based nanocomposites.

The combination of polymers and inorganic materials represents a new strategy to obtain a special class of hybrid systems, termed *polymeric nanocomposites,* with the specific properties required by a wide range of applications in biotechnology, nanomedicine, catalysis, chemical sensors, actuators, electromagnetic interference shielding and microwave absorbing etc. One of the main challenges of our research in the field of polymer based nanocomposites was to synthesize hybrid combinations that keep or enhance the best properties of each of the components while eliminating their particular limitations.

Among the nanocomposite materials we focused on ***polymer/magnetic nanocomposites*** because they provide specific properties and advanced processing capabilities with dual-mode manipulation controlled by a magnetic field and through an appropriate design of surface properties. Nanocomposites based on magnetic nanoparticles and biocompatible polymer and block copolymer present a twofold interest. First of all these materials rise fundamental challenges concerning new specific processes and phenomena induced by the nanostructure, specific molecular interactions, interface effects and phase transitions in complex supramolecular systems. The major interest is however their applicability in biotechnology and nanomedicine which undergo an explosive increase in the last decade. We combine the attractive properties of the polymer such as structural stability, elasticity, the simple procedures for polymorphic synthesis, the corrosion resistance with the properties of magnetic nanoparticles to get new multifunctional materials.

In the last few years our research has been focused on ***smart magnetic nanocomposites able to modify their structure and to respond to some environmental stimuli (temperature, pH)***. Smart magnetic materials are obtained by mixing the magnetic nanoparticles with smart polymers, which

means polymers which undergo relatively large and sharp physical changes with small continuous changes of some environmental parameters.

Magnetic micro/nanogels obtained by encapsulation of magnetic nanoparticles into stimuli responsive polymers acting as clustering agents, represent good candidates for biomedical applications and high gradient magnetic separation process because they fulfill important requirements such as: superparamagnetic behaviour, high saturation magnetization/large magnetic moment, response to moderate magnetic fields, rich in surface functional groups. Moreover, the potential application of stimulus responsive magnetic nanogels in drug delivery has emerged as one of the most significant trends in nanomedicine.

On national level, the researches in the field of polymers and hybrid polymer-inorganic nanoparticles are in full development. Research teams of other institutions such as the Institute of Macromolecular Chemistry Petru Poni Iasi, National R&D Institute for Materials Physics Bucharest, University „Politehnica" Bucharest are active in this area, however do not refer to *magnetically responsive* polymeric nanocomposites. ***To our best knowledge, there are no other Romanian groups working on the topic of magnetic micro/nanogels and their applications.***

The specific objectives of the research:

1) Development of synthesis methods for nanocomposites based on magnetic nanoparticles and polymers or block copolymers with tailored properties;

2) Synthesis of new functionalized magnetic nanocomposites based on polymers (conjugated polymers, responsive polymers) and magnetic nanofluids;

3) Determination of physical-chemical properties of nanocomposites based on magnetic nanoparticles and polymers or block copolymers;

4) Controlled and reproducible synthesis of smart nanocomposites based on magnetic nanoparticles and stimuli-responsive biocompatible polymer or block copolymer;

5) Functionalization of smart magnetic materials based on polymers in order to extend their applicability;

6) Assessment of the potential applications of functionalized magnetic nanocomposites in biotechnologies and nanomedicine;

7) Dissemination of results: articles in ISI quoted journals, national and international conferences in the field;

8) Integration of the national research activity in the field of novel nanostructured polymeric composites in the framework of the European research program FP7 and European technological platforms;

9) Development of partnership with European research institutes in the framework of international projects.

These objectives were fulfilled in the framework of several national and international research projects, through a trans-disciplinary partnership of scientists from INCDTIM and other

institutes and universities combining excellence in different scientific areas: physics, chemistry, materials science and engineering, nano- and biotechnologies.

National research projects: ***9 projects coordinated by INCDTIM*** (1 project – program MATNANTECH, 2 projects –program CERES, 1 project – program CEEX-MATNANTECH, 1 project – program CEEX-Modul III, 1 project – program CEEX-ET, 2 projects – PNII, 1 project POS-CCE O2.1.2)***. We have to underline that all the project proposals made by the research group from INCDTIM in the field of polymer based nanocomposites in the framework of the national competitions (period 2001-2010) have been accepted.***

International research projects: ***3 projects***

The research activity performed in INCDTIM in the field of polymer based nanocomposites was appreciated by the international scientific community and as a result the research group from INCDTIM participate as a partner in ***2 projects financed by the European Community: FP6-NMP- NoE 2004-2008 No. 500361-2 NANOFUNPOLY „Nanostructured and Functional Polymer-Based Materials and Nanocomposites"*** and ***FP7-NMP- Large 2009-2013 No. 229335 MAGPRO²LIFE-„Advanced Magnetic nanoparticles deliver smart Processes and Products for Life".*** A bilateral research project in partnership with Institute of Materials Jean Rouxel (IMN) Nantes, France was managed in the field of polymer based nanocomposites (2005-2006).

The main research activities performed:

- **i)** Development of innovative methods for synthesis of polymers with special properties and nanocomposite materials based on polymers and magnetic nanoparticles/magnetic nanofluids
- **ii)** Preparation of new functionalized magnetic nanocomposites with tailored electrical and magnetic properties based on conducting polypyrrole and magnetic nanofluids
- **iii)** Preparation of smart nanocomposites with controlled architecture based on magnetic nanoparticles and stimuli-responsive polymers (core-shell systems, macro and microgels)
- **iv)** Preparation of new recyclable organic catalysts based on functionalized magnetic nanostructures
- **v)** Complex characterization of functionalized magnetic nanocomposites: nanostructure-properties relationship, responsive properties to external stimuli, biocompatibility
- **vi)** Investigation of specific interactions between the functionalized magnetic nanocomposites and biomolecules (proteins, peptides) as well as selected drugs
- **vii)** Testing the potential applications of functionalized magnetic nanocomposites for magnetic separation of biomolecules, targeted drug delivery and as new recyclable organic catalysts.

The main results achieved in the field of were published, presented at scientific meetings and included in patents applications: ***11 articles in ISI journals, 16 articles in other journals and 3 book chapters published abroad, 2 patents applications.*** We mention that from the 27 published articles, ***9 articles have co-authors our collaborators from abroad.***

The main results may be structured as follows:

1. Innovative scientific results:

- ***New synthesis methods:***

- Laboratory procedure for the synthesis of magnetic nanocomposites based on magnetic nanofluid and functionalized polypyrrole (patents applications RO-A/00401–15.07.2008, RO-A/00997-27.11.2009)
- Microwave assisted synthesis method of hybrid nanostructures based on magnetic nanoparticles and polylactones;
- Laboratory procedure for the synthesis of smart nanocomposites based on magnetic nanoparticles and polymers /copolymers responsive to external stimuli (core-shell systems, macro and microgels).

- ***Products:***

- New hybrid nanostructures based on magnetic nanofluid and functionalized polypyrrole (patent application RO-A/00997-27.11.2009)
- Core-shell type hybrid nanostructures based on magnetite and biocompatible polymers (poly-caprolactone, poly-lactic acid, poly-hydroxyethyl methacrylate, poly N-isopropylacrylamide);
- Smart magnetic microgels based on magnetic nanofluid and stimuli responsive polymers (poly N-isopropylacrylamide, poly-acrylic acid);
- New recyclable organic catalysts based on functionalized magnetic nanostructures.

2. Scientific results with applications in biotechnology and nanomedicine:

- Functionalized magnetic microgels could be used for new technologies of magnetic separation that can be taken by the pharmaceutical industry; functionalized magnetic microgels, can be applied by economic agents manufacturers of laboratory reagents used for protein separation sets, cell separation and other biomaterials separations.

  The tests of magnetic separation of biomolecules using the magnetic microgels produced by the research group from INCDTIM were performed by the FP7 MagPro2Life project partners (MERCK, Karlsruhe Institute of Technology) and demonstrate that these materials have very good properties suitable for magnetic separation application. These materials will be considered for testing in the magnetic separation pilot lines planned as a final objective of FP7 project.
- Functionalized magnetic nanocomposites based on biocompatible polymers can be used in nanomedicine as new magnetically targeted carriers for therapeutic agents, hyperthermia treatments and for diagnostic (MRI).
- New recyclable organic catalysts based on functionalized magnetic nanocomposites can be used for various chemical reactions with significant impact in chemical, pharmaceutical or

cosmetic industry related to the reduction of production costs, waste materials, omission of toxicity issues and easy processability.

3. Results of socio-professional impact:

- Creation of 7 working places in INCDTIM for young researchers and senior researchers;
- Increase of the research performances by purchase of new equipments: X-ray Photoelectron Spectrometer (XPS), AFM/STM microscope working under ultra high vacuum, SQUID magnetometer;
- Development of a new chemistry laboratory, well equipped to satisfy the highest requirements of the research work in the field of advanced materials synthesis;
- Increase the expertise level and visibility of the research activity of INCDTIM in the field of advanced materials and innovative processes;
- Training of young researchers in the following areas: advanced synthesis methods, materials science, biotechnology;
- Increase of the participation of the Romanian researchers to the international projects;
- New bilateral projects with partner European institutions;
- Attracting and involving researchers from abroad in Romanian research projects;
- Integration of the national research activity in the field of novel nanostructured polymeric composites in the framework of the European research program.

4. Collaborations and partnerships with other prestigious institutions in the country and abroad

- ***National collaborative partnerships:*** Center for Fundamental and Advanced Technical Research-Romanian Academy-Timisoara Branch, National Institute R&D for Materials Physics Bucharest, Babes-Bolyai University Cluj-Napoca.
- ***International partnerships****:* Institut fur Chemie, Humboldt University Berlin; Institute of Polymer Science, CSIC Madrid; Institute des Materiaux Jean Rouxel, Nantes; Solae Denmark, MERCK- Germany, ETH Zurich, Switzerland; Karlsruhe Institute of Technology (KIT), Karlsruhe Germany; Universitätsklinikum Erlangen - Section for Experimental Oncology and Nanomedicine(SEON) Erlangen, Germany.

Cluj-Napoca, December 14 , 2011.

INCDTIM's Top Management

and R&D team leaders