Sixth Framework Programme
EC-INCO-CT-2005-016414

Project No. **EC-INCO-CT-2005-016414**

Project acronym: **MISSION**

Project Title: **Centre of Multifunctional Materials and New Processes with Environmental Impact**

Instrument: **Specific Support Action**

Thematic priority**: Nano, Citizens**

PUBLISHABLE FINAL ACTIVITY REPORT

Period covered: **from May 1st, 2005 to April 30th, 2008**

Date of preparation: **June 2008-06-09**

Start date of project: **May 1st, 2005**

Duration: **36 months**

Project coordinator name: **Prof. DSc. Konstantin Hadjiivanov**

Project coordinator organization name: **Institute of General and Inorganic Chemistry, Bulgarian Academy of Sciences**

Table of Contents

1. Project execution

1.1 Summary Description of Project Objectives

The **Centre of Multifunctional Materials and New Processes with Environmental Impact (MISSION)** is one of the seven Bulgarian Centres of competence established as a result of the EC call: "Promotion of Co-operation with Associated Candidate Countries: Reinforcement of the Associated Candidate Countries' Research Capacities" from the Specific Support Action "Integrating and Strengthening the European Research Area" (FP6-2004-ACC-SSA-2).

The main goal of **MISSION** is to establish at the Institute of General and Inorganic Chemistry (IGIC) an innovative leading Centre of Development and Management of Multifunctional Materials and New Processes with Environmental Impact based on cross-links science-education-industry-society. The specific mission of **MISSION** is to train a new generation of young scientists who will then transfer the obtained knowledge to their new working places.

The specific objectives of **MISSION** are:

1. Reorganization of IGIC and focusing its activities on the environmental aspects of multi-functional materials and new processes;
2. Enhancement of the research capabilities of IGIC for the development of environmentally oriented multifunctional materials and new processes;
3. Expansion of the contacts between IGIC and leading research institutions in Europe;
4. Promotion of the careers of young scientists and maintaining a high educational level;
5. Dissemination of knowledge to the scientific community, industry and society.

The final objective of **MISSION** is the continuous development of the Centre after the end of the project in order to meet the specific current demands of the society.

1.2 Contractors Involved

The Centre **MISSION** was established on May 1st, 2005 at the Institute of General and Inorganic Chemistry (IGIC) of the Bulgarian Academy of Sciences. IGIC is one of the principal and oldest chemical institutes of the Bulgarian Academy of Sciences. The activities of the institute include basic and applied research, consultancy, industrial practice and teaching in three main research areas: inorganic materials science, chemical analysis and sorption & catalysis. The website of IGIC is http://www.igic.bas.bg.

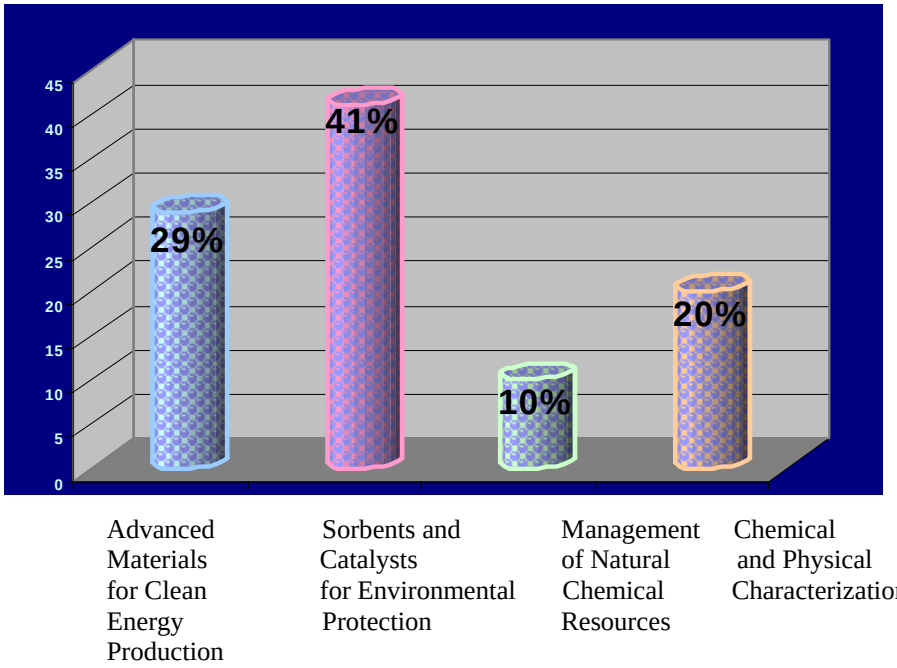
1.3. Co-ordinator Contact Details

The Project coordinator is the Director of IGIC Professor DSc Konstantin Hadjiivanov (tel.: +35929793598, fax: +35928705024, e-mail: director@svr.igic.bas.bg), http://www.igic.bas.bg/kux.html.

1.4. Work Performed and Results Achieved

The work on the project is divided into 9 workpackages (WPs): (i) Project Management; (ii) Materials for Clean Energy Production; (iii) Sorbents and Catalysts for Environmental Protection; (iv) Sustainable Utilization & Management of Natural Chemical Resources; (v) Chemical & Physical Characterization of Multifunctional Materials. Metrological Control and Standardization; (vi) Strengthening of the International Co-operation; (vii) Strengthening of Young Scientists Qualification; (viii) Public & Industry Relations. Dissemination of Knowledge; (ix) Closing Conference.

The total number of scientists and PhD students included in the implementation of the MISSION project is 59. The distribution of the research potential within the priority topics is as follows:



The activities of the Centre are:

1.4.1. Effective management

The effective management included regular meetings of the Steering committee. Special efforts were focused on the upgrade of the equipment and elaboration of rules for its efficient use. Four meetings of the Steering committee with the participation of the members of the Advisory board were carried out in this period. The suggestions of the Advisory Board members during the first three meetings were taken into consideration. On the fourth meeting evaluation of the entire work was made and directions for the future development of the Centre were discussed.

1.4.2. Reorganization of the Institute of General and Inorganic Chemistry

In order to focus the research activities on the environmental aspects of multifunctional materials and new processes, structural reorganization of the Institute was made in order to allow covering the areas of the thematic WPs of **MISSION**.

1.4.2.1 Upgrade of the equipment

Three scientific instruments were purchased for precise characterization of multifunctional materials:

1. A Bruker D8-Advance X-Ray powder diffractometer. D8 Advance is equipped with a highly precise theta/theta goniometer and an energy-dispersive SoI-X detector. The new diffractometer allows qualitative and quantitative phase analysis, structure determination and refinement, crystallite size and microstrain determination

2. A SOLAAR M6 atomic absorption spectrometer from Thermo Elemental. The spectrometer is equipped with high quality double beam optics (Stockdale system), an Echelle monochromator and sealed optics against corrosive vapors ingression. The new spectrometer allows precise micro-trace analysis of multifunctional materials.

3. Solid state nuclear magnetic resonance spectrometer Bruker Advance 600 MHz II (in co-ownership with other Bulgarian research institutions). The new spectrometer allows local structure determination and elucidation of its impact on the properties of a wide range of technologically important materials. This is the first solid-state NMR in Bulgaria.

1.4.2.2. Promoted qualification of young scientists

The work performed under this objective was in three main directions:

(I) Opening PhD positions.

Six PhD positions were opened within the framework of the **MISSION** project. The new PhD students started their activities on June 01, 2005. They already prepared the draft versions of their theses. The PhD theses are focused on:

- Layered lithium-nickel-manganese oxides for cathode materials in lithium ions cells;
- Preparation, chemical and structural modification of cathode materials for solid oxide fuel cells;
- Storage catalysts for NOx neutralization;
- Gold catalysts for environmental protection;
- Ecological chemical technologies in the sea salt production;
- Development of validated methods for the atomic absorption spectrometric determination of trace elements in waters.

The PhD students are: MSc. Meglena Yoncheva, MSc. Sonya Ivanova, MSc. Angelina Mihailova, MSc. Hristo Klimev, MSc. Antonina Kovacheva and MS Eng. Alexander Petrov.

The supervisors are the following WP leaders: Assoc. Prof. Dr. E. Zhecheva, Assoc. Prof. Dr. R. Stoyanova, Assoc. Prof. Dr. Velin Nikolov, Assoc. Prof. Dr. Plamen Stefanov, Assoc. Prof. Dr. Anton Naydenov, Prof. DSc. Konstantin Hadjiivanov, Assoc. Prof. Dr. Radostin Nikolov, Assoc. Prof. Dr. Stefka Tepavitcharova, Assoc. Prof. Dr. Ivan Havezov and Prof. DSc. Elisaveta Ivanova.

(II) Training of young specialists

Several young scientists were appointed at IGIC and were trained in the fields covered by **MISSION:** (i) MSc. Ekaterina Popova (since July 1st 2005) – preparation methods of materials for lithium ions cells; (ii) Sc. Zhelio Andreev (November 21st 2005 – July 10th 2006) – preparation methods of electrolyte materials for solid oxide fuel cells; (iii) MSc. Petar Zvetkov (since July 1st 2006) – XRD characterization of inorganic solids; (iv) Dr. Albena Bachvarova (since July 1st 2005) – preparation of sorbents and catalysts for environmental protection; (v) MSc. Boriana Kotzeva (since June 1st 2005) - chemical analysis of fluid inclusions in Bulgarian minerals. Theoretical and practical training activities were organised for two IGIC young specialists on the case of ASAREL-MEDET Cu-Mo mine environment. The interest was directed towards establishment and evaluation of the environmental affect of the mining activities and in methods for environment remediation.

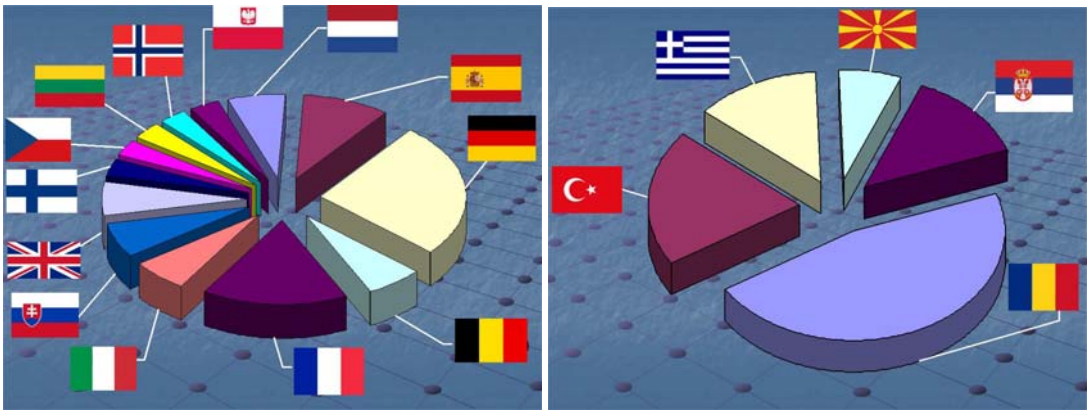
(III). Increase of the qualification of the young scientists

This was achieved by organizing several different courses for three target groups: (i) new PhD students, (ii) recruited young scientists and (iii) young scientists from IGIC. The courses were (i) specialized scientific courses and (ii) courses for skill improvement, e.g., English language courses and computer skill courses. The *Course of computational chemistry*, where prominent European scientists in the field were invited as speakers, involved a larger audience - students from different Universities and Institutes from the whole country.

Important for the career of the young researchers was their participation at scientific meetings (39 participations in the country and 26 participations abroad) and research stays in leading European centres (11 visits).

1.4.2.3. International Cooperation

The international cooperation was promoted by (i) inviting prominent European scientists for short-term (18) and long-term (2) visits as well as research visits of **MISSION** participants in leading European laboratories (11 short-term and 8 long-term). As an illustration, the chart diagram shows schematically the established contacts with leading European scientists, as well as with scientists from research institutions in the Balkan region:



Thematic databases covering the **MISSION** priorities were created. A collection of Bulgarian and EU regulatory issues for standardization of inorganic materials was done. Data bases on Bulgarian SMEs and firms dealing with materials production and/or trade were created. All databases and collections are put at disposition of the members of the MISSION project. The collected information was used to map the scientific institutions in Europe carrying out research on the thematic areas in question. In addition, a critical analysis concerning the research efforts in Europe and the Balkan region was made.

The most significant conferences and meetings in relation with the priority topics of the **MISSION** Centre were attended by both senior and young scientists, distributed by topics as follows:.

Topic: Materials for Clean Energy Production

- International Meeting on Lithium Batteries (IMLB), June 18-23, 2006, Biarritz, France;
- 8th International Conference Advanced batteries and accumulators (A.B.A-8, June 3rd-7th, 2007, Brno University of technology, Czech Republic;
- 3-rd International Conference on Green and Sustainable Chemistry (GSC-3), July 1-5, 2007, Delft University of Technology;
- World Hydrogen Technologies Convention 2007 (WHTC), 4-7.11.2007, Montecatini Terme – Italy ;
- International Conference on Coherent and Nonlinear Optics (ICONO 2007) collocated with International Conference on Lasers, Applications, and Technologies (LAT 2007), May 28-June 1, 2007

Topic: Sorbents and Catalysts for Environmental Protection

- 4th EFCATS School on Catalysis CATALYST DESIGN – FROM MOLECULAR TO INDUSTRIAL LEVEL, September 20-24, 2006 in Russia (Tsars Village, St. Petersburg);
- 17th International Vacuum Congress and 13th International Conference on Solid Surfaces, July 2-6, 2007, Stokholm, Sweden;
- EUROPACAT VIII, 26-31.08.2007, Turku/Åbo, Finland.
- *Topic: Sustainable Utilization and Environmentally Friendly Management of Natural Chemical Resources*
- Workshop "Livable Cites", 10th -12th May, 2006, Bourgas, Bulgaria;
- 12th International Symposium on Solubility Phenomena and Related Equilibrium Processes (12th ISSP), 23-28.07.2006, Freiberg, Germany;
- 6th ANQUE, International Congress of Chemistry on the Topic of Chemistry and Sustainable Development, 5-7th December 2006 Puerto de la Cruz, Tenerife (Spain);
- 3rd International Symposium Recent Advances in Trace Elements Research, 16th -19th May, 2007, Santiago de Compostela, Spain.

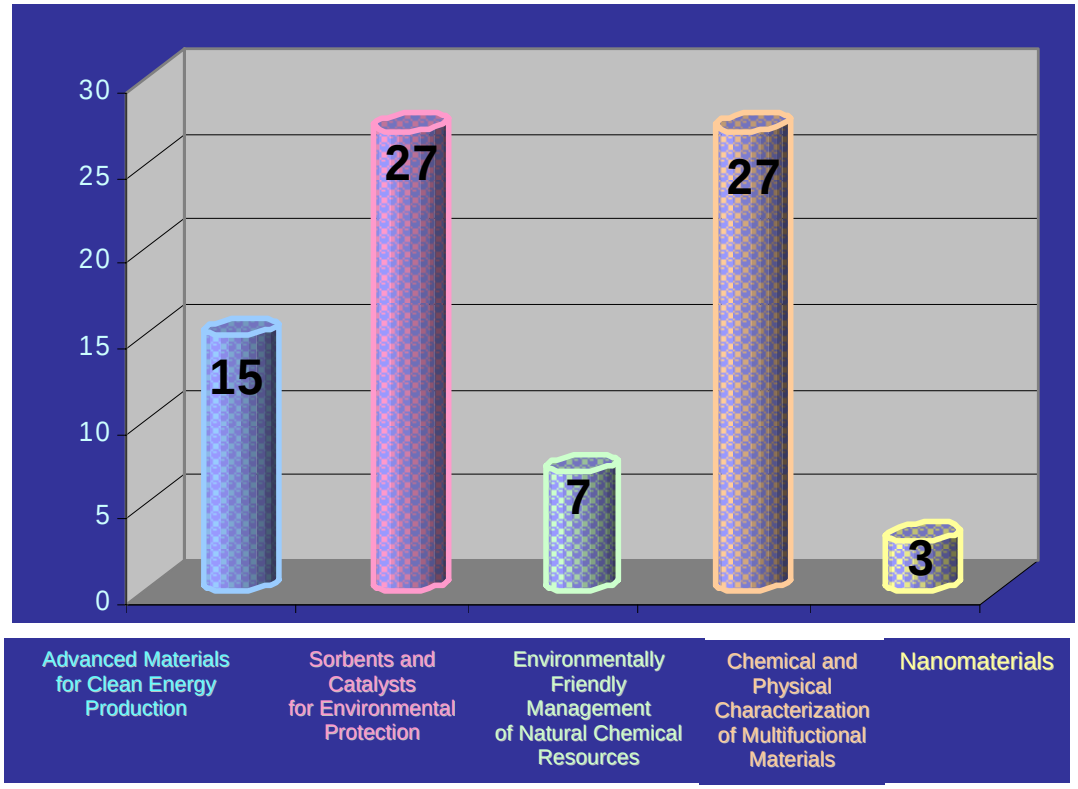
Topic: Chemical and Physical Characterization of Multifunctional Materials: Metrological Control and Standardisation

- International Congress on Analytical Sciences, 25-30.06.2006, Moscow, Russia;
- Training in Metrology in Chemistry, 6.11.-8.11.2006, Sofia, Bulgaria;
- EUROANALYSIS XIV, 9-14.09.2007, Antwerp, Belgium;
- 4th Black Sea Basin Conference on Analytical Chemistry, 19-23 September, 2007, Sunny Beach, Bulgaria;
- Waste Management, Water Pollution, Air Pollution, Indoor Climate, 14 – 16 October 2007, Arcachon, France

Scientific meetings with general scope were also attended:

- NTNE Nanotech Northern Europe 2007, Congress and Exhibition Helsinki, Finland, March, 27-29, 2007;
- 3rd International Conference on Amorphous and Nanostructured Chalcogenides Fundamentals and Applications, July 2-6, 2007, Brasov, Romania;
- 5th International Conference of the South-East European Chemical Societies ICOSECS, September 10-14, 2006, Ohrid, Macedonia.

The distribution of the conference participations within the thematic priorities is as follows:



1.4.3. Organization of Scientific Meetings:

1.4.3.1 The Workshop SIZEMAT (*Size-Dependent Effects in Materials for Environmental Protection and Energy Application)* took place in Varna from 25 to 27 May 2006. The participants, 108 persons, were mostly young scientists from the Balkan region. Prominent European scientists accepted the invitation to hold the invited lectures. A book of abstracts was prepared. A special issue of the *Journal of Materials Science* contains 15 selected contributions from the presented at the Workshop. The website of the workshop is http://sizemat.igic.bas.bg.

1.4.3.2 The METECOMAT Workshop *(Ecomaterials and Processes: Characterization and Metrology)* was held in April 19 - 21, 2007, in Plovdiv, Bulgaria. The participants, 88 persons, were mainly young scientists from the Balkan region. The invited speakers were prominent European scientists. The abstracts were published in a separate book while elected papers will soon appear in a special issue of the journal *Environmental Chemistry Letters*. The web site of the workshop is http://metecomat.igic.bas.bg.

1.4.3.3 The **MISSION** Closing Conference "*Multifunctional Materials and New Processes with Environmental Impact*" was held in Bankya in April 03-05, 2008. The aim of the Conference was to present and discuss the project activities; to highlight and assess the scientific achievements and future trends of the **MISSION** Centre. The young **MISSION** participants presented their scientific achievements in the whole period of project duration.

1.4.4. PR activities and Contacts with Industry:

The Round-table *European funds – basis for sustainable relations Science – Industry – Society in the field of materials science in Bulgaria* took place in February 2007 with participation of representatives of the scientific community, small and medium-size enterprises, governmental and non-governmental organizations and mass media, experts from the Ministry of Finance, the Ministry of Economy and Energy, the Bulgarian Small and Medium-size Enterprises Promotion Agency as well as from a private consulting company.

Two Round-table discussions on the *Protection and use of Black Sea natural resources* with a wide range of local and regional stakeholders were organized. The collaboration with the Municipalities of Bourgas and Pomorie - cities situated at the Bulgarian Black Sea, were established with the aim to elaborate a Program for socio-economic development of the Bourgas Municipality in the next 7-year period.

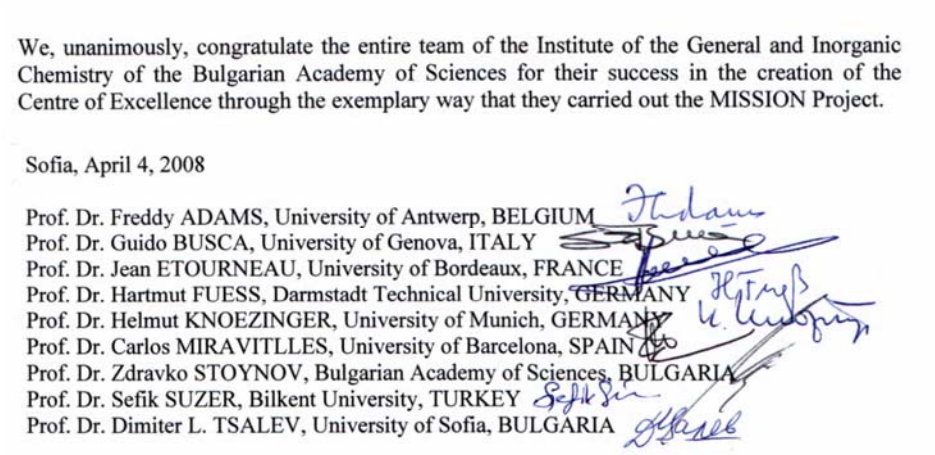
The Round-table *Challenge Materials for Sustainable Society Development* with emphasis on the future prospects of the **MISSION** Centre took place in the afternoon session of the Closing Mission Conference (April 2008).

Series of PR activities were performed, e.g., advertising the **MISSION** project in newspapers, TV and radio emissions, exhibitions, a.o.

1.5 End Results

As a result of the enhanced contacts with European scientists and industry, the number of different projects prepared and submitted with participation of IGIC increased. In particular, a new Centre for transfer of knowledge, **TRANSMISSION**, based on **MISSION** achievements and complementing its activities, was established at the institute in the framework of the PHARE programme.

The members of the Advisory Board signed a Statement that the goals of the project have been successfully achieved and the Centre of Competence on Multifunctional materials and new processes with environmental impact created at IGIC within the **MISSION** project will secure the continuity of the high level of research reached as a result of the successful project.



We, unanimously, congratulate the entire team of the Institute of the General and Inorganic Chemistry of the Bulgarian Academy of Sciences for their success in the creation of the Centre of Excellence through the exemplary way that they carried out the MISSION Project.

Sofia, April 4, 2008

Prof. Dr. Freddy ADAMS, University of Antwerp, BELGIUM
Prof. Dr. Guido BUSCA, University of Genova, ITALY
Prof. Dr. Jean ETOURNEAU, University of Bordeaux, FRANCE
Prof. Dr. Hartmut FUESS, Darmstadt Technical University, GERMANY
Prof. Dr. Helmut KNOEZINGER, University of Munich, GERMANY
Prof. Dr. Carlos MIRAVITLLES, University of Barcelona, SPAIN
Prof. Dr. Zdravko STOYNOV, Bulgarian Academy of Sciences, BULGARIA
Prof. Dr. Sefik SUZER, Bilkent University, TURKEY
Prof. Dr. Dimiter L. TSALEV, University of Sofia, BULGARIA

Facsimile of part of the Letter of Statement of the Advisory board

1.6 Project Website

An Internet website of **MISSION** was set, where the progress of the project work could be monitored: http://mission.igic.bas.bg/. A special logo of **MISSION** was designed. At the website the programs and the lectures of the **MISSION** courses ("***Computational Chemistry", "Adsorption Methods for texture analysis",*** and ***"Atomic Absorption Spectroscopy methods")*** have been announced. Userful information about the activities of the **MISSION** ***Centre*** was also available at the **MISSION** website.

2. Dissemination and Use

2.1. General Considerations

Various research and popular products developed in the frame of the MISSION project were specifically tailored to raise the impact of the science on the Bulgarian society.

At first place the PhD thesis programs and topic courses dedicated to prepare young specialists for high quality researches in the specific fields corresponding to the research workpackages should be mentioned.

Besides, there was a strong knowledge and information dissemination element in this project aimed to generate useful contacts between Bulgarian, Balkan and European research societies by the two thematical workshops organized, by the oral and poster presentations at many European scientific forums, by long-term and short-term specialization of young scientists from IGIC at leading Laboratories and Centers in Europe.

To make the information about MISSION achievements available to a wider audience, several Round-table discussions were organized, thus popularizing products developed in the

frame of the project. One Round-table discussion conwas dedicated to the relations between the governmental authorities, science and industry.

The active dissemination strategy enabled us to reach to the general public by the following media:

- Actual information about MISSION activities appeared regularly at the project web site;
- Publications in the Bulletin of the Bulgarian Academy of Sciences – introducing new equipment at the Institute obtained with the financial support of the project;
- Posters and broshures were presented and distributed at commercial and technical exhibitions showing the ability of IGIC to solve problems of the industrial production;
- Several publications appeared in national and regional newspapers destined to the general public and aiming explanation of the role of the MISSION project for enhancing the level of research and the results of this research which could be implemented into the industry through the introduction of new knowledge-based products, materials and technologies;
- Electronic media – radio and television emissions were the most powerful tool to make many people familiar with the project activities and results.

2.2. Specific Aspects

The specific aspects of dissemination and use are presented below:

1) MISSION *Internet web-site* (*http://mission.igic.bas.bg*);
2) *Information in the Internet* about the workshops (*SizeMat* and *MetEcoMat*) using corresponding links (*http://sizemat.igic.bas.bg/; http://metecomat.igic.bas.bg/*);
3) *The programs and the lectures* of the organized MISSION courses ("*Computational Chemistry", "Adsorption Methods for texture analysis" and "Methods for environmental analysis")* are accessible at the MISSION *Internet website* (*http://mission.igic.bas.bg*)*;*
4) *Information* about the MISSION activities appeared in the *Information Bulletin of IGIC* (*http://www.igic.bas.bg*): Bulletin25/2006, Bulletin26/2006, Bulletin27/2006, Bulletin28/2006, Bulletin29/2006/, Bulletin34/2007, Bulletin36/2007;
5) *Four publications* in the *Informational Bulletin of the Bulgarian Academy of Sciences*:
    a) *http://www.bas.bg/basnews/bulletin/Bul104.pdf* (page 18);
    b) *http://www.bas.bg/basnews/bulletin/Bul106.pdf* (page 14);
    c) *http://www.bas.bg/basnews/bulletin/Bul110.pdf* (page11);

d) *http://www.bas.bg/basnews/bulletin/Bul118.pdf* (page 7).

6) Press activities of the MISSION Coordinator, Prof. DrSc K. Hadjiivanov, interviews for the national newspapers *"Novinar", „Duma" and „Sega":*

a) *"Novinar"* - 21.11.2007 http://www.novinar.net/?act=news&act1=det&stat=center&mater=MjQ0MjszNg==;

b) *„Duma"* – 05.12.2007 http://www.duma.bg/2007/1207/051207/index.html;

c) *"Sega"* - 18.02.2008 http://www.segabg.com/online/article.asp?issueid=2889&sectionid=28&id=0001301;

d) *"Novinar* – 08.04.2008 – http://www.novinar.net/?act=news&act1=det&stat=center&mater=MjYxNzsyMQ==;

e) *Interview* with Prof. DrSc K. Hadjiivanov and Prof. Etourneau for "Nova" national television – 04.04.2008 - www.neterra.tv/bg.

7) *Interviews* of the MISSION project Coordinator, Prof. K. Hadjiivanov, concerning the Round-table on theme *"The European Funds – basis of new and sustainable relations science – industry-society in the field of the materials science in Bulgaria*" (Sofia, 23.02.2007):

a) *Record of interview* with Prof. DSc. Konstantin Hadjiivanov, *on 22.02.2007* for the Bulgarian National Radio, program *"Hristo Botev"*;

b) *Record of interview* with Prof. Konstantin Hadjiivanov, on *23.02.2007* for the Bulgarian National Radio, program *"Horizont"*;

c) *Reportage* emitted by the "Alma Mater" Radio about the Round-table: *Record of interview with* Prof. K. Hadjiivanov for the Bulgarian National Radio, *on 01.11.2007,* concerning IGIC and MISSION activities on occasion of the "Bulgarian Academic day";

8) *Record of interviews with* Prof. K. Hadjiivanov and Prof. J. Etourneau *on 03.04.2008* for the Bulgarian national television "NOVA" on the achievements of the MISSION project.

9) *Presentations of the invited lecturers at the Round-tables*

10) *Record of the Round-table discussions*

11) Poster presenting the MISSION activities at the Launching Conference on theme *"Seventh Framework Programme for research, technological development and demonstration activities"*:
12) *Data bases* on Bulgarian SMEs and firms dealing with materials.