

ADVANCES IN BULGARIAN SCIENCE



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52 A. G. M. Kimitriv Blvd
1125 Sofia, Bulgaria,
Phone: +359 2 817 38 62
http: www.nacid-bg.net
e-mail: advances@nacid-bg.net

Editorial board:

Vanya Grashkina, Klga Racheva,
Yana Panova, Kostadin Tonev,
Milen Angelov, Tzvyatko Stoyanov
Lyudmila Velkova

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Kear Ladies and Gentlemen,

We present to you the first issue of the bulletin „Advances in Bulgarian Science“ edited by the National Centre for Information and Kocumentation (NACIK).

Science has developed so rapidly over the last century that even the most motivated scientists cannot follow the state of the art in research areas different from their own.

The advances of contemporary science during the last decades are so overwhelming that they can make the broad community believe the fundamental scientific problems are already solved, and the future challenges are not so important. However, we are now facing even more challenging research areas and discoveries in all fields of science.

The nature of science is global, not national or local. Science has neither geographical boundaries, nor state borders. Consequently it has become more than ordinary for scientists from different countries to exchange ideas and maintain joint research activities. Kevelopment of electronic communications facilitates these processes as never before.

Fortunately Bulgaria has long lasting traditions in scientific researches and research exchange.

The main objective of this bulletin is to rise the awareness of the international scientific community about the advances of Bulgarian science and about the Bulgarian researchers who, despite the recent challenges to the national scientific system, are furthering the country's traditions in science with their expertise and exceptional motivation. For this they deserve the corresponding respect and decent prospects for their future career.



Vanya Grashkina,

Executive Kirector



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National Centre for Information and Documentation

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NATIONAL SCIENTIFIC PROGRAMMES WITH EUROPEAN DIMENSIONS

HIGH LEVEL COMPUTATIONAL MODELING – A SUCCESSFUL APPROACH TO UNDERSTANDING THE BEHAVIOR AND DESIGN OF NEW MATERIALS

Georgi N. Vayssilov

Faculty of Chemistry, University of Sofia, 1126 Sofia, Bulgaria,
web site: <http://www.chem.uni-sofia.bg/depart/ochem/catalysis/>
e-mail: gnv@chem.uni-sofia.bg

The development of new materials with extensive applications not only in modern technologies, but also essentially in all fields of human life is one of the main achievements of scientific research in the last decades. The progress in this field has been promoted by the crucial advances in the fundamental experimental characterization techniques, reaching already the single molecular and atomic levels, and by the methods for reproducible preparation of ordered molecular, supra-molecular or atomic aggregate structures, as well as for their controlled manipulation and transformation. These modern experimental approaches make use of a wide variety of physical and chemical treatments, laser, molecular and ionic beam techniques, various spectroscopic and microscopic methods, etc. Contemporary computational approaches for modeling and simulation of the molecular, cluster, and materials structure and properties have also a substantial contribution to the development of new materials. During the last decade, these methods have become feasible for realistic applications to systems of practical interest essentially owing to the rapid progress in computers and fast development of efficient and reliable computational methods and procedures. The importance of the later achievements was acknowledged by the Nobel Prize in Chemistry (1998) to Walter Kohn and John Pople [1] for the development of computational methods in quantum chemistry (QC) and particularly for the den-

sity-functional (KF) theory. Nowadays, such computational modeling provides not only insights towards the understanding of the nature, structure, and behavior of the existing systems, but also allows simulation of new imaginary species and materials that plays a key role in the design and tailoring of new materials with pre-defined properties. This fascinating ability of the computational methods to contribute to the elucidation of mechanisms and origins of the chemical and physical processes on the molecular and atomic levels, and at the same time to assemble, test and upgrade virtual materials in order to acquire species with specific desired features, was the reason for our keen interests in the field of computational chemistry.

The Laboratory of Organic Catalysis [2] at the Faculty of Chemistry, University of Sofia, was established in 1958 by Professor C. Kimitrov. For more than 40 years, the research activities in the laboratory have been focused on the chemical and catalytic properties of zeolites and related micro- and mesoporous materials, and their applications in chemical industry. Zeolites are a class of crystalline aluminosilicate materials with precisely defined structure of internal pores and cavities with diameter below 1.5 nm (Fig. 1) and, for this reason, they are also called molecular sieves since these dimensions fit to the size of molecules containing from one to several dozens of atoms. Lately, this class has been extended by crystalline

microporous materials of different compositions, particularly phosphates, as well as by a new generation of well ordered amorphous materials with pores wider than 2 nm, the so-called mesoporous materials. Due to their peculiar structure and specific sorbent and catalytic properties, molecular sieves have been traditionally used in petrochemical and detergent industry. However, recent advances in the synthesis of new structures and compositions and, particularly, the subsequent tailored modification of these materials extended considerably the areas of application of zeolites and related materials not only to other branches of chemical industry, but mainly to various hi-tech applications where they are used as components in electronic, optical, sensor, etc. devices. The productivity, achievements and international recognition of Bulgarian scientists in the field of micro- and mesoporous materials ensured their outstanding position, as compared to other fields of natural and technical sciences. One can clearly see that zeolite research is among the leading research fields; according to current information from Thomson ISI, five [3-7] of the top eight most cited Bulgarian papers in chemistry concern studies on zeolites. In order to facilitate the further successful research and international cooperation in this area, we are organizing an International Symposium on "Catalytic Processes on Advanced Micro- and Mesoporous Materials", which will take place in Nessebar, Bulgaria, September 2-5, 2005 [8].

Due to the interesting properties and the promising future of the microporous and mesoporous materials and the abilities of the computational method for materials modeling and design, we directed our research mainly on computational studies of zeolites and similar materials in the area of overlap of the computational and materials chemistry. In particular, we focus on investigations of the structure, spectral features and chemical properties of zeolites functionalized with metal cations, embedded metal clusters or organic molecules. The immobilization of very small transition metal species or functional organic compounds in suitable micro- and mesoporous molecular sieves with nano- and subnano-size pores is performed to provide reliability, efficiency and controlled properties of the obtained complex

materials. In order to take advantage of the design of such new materials with desired properties, we also carry out experimental preparation and characterization of zeolite-immobilized photosensitive organic compounds with defined spectral and optical properties. Here, I will describe some of our recent achievements. Essentially, all studies have been performed in close cooperation with several partner groups working either experimentally or theoretically. All theoretical studies on zeolites and metal cluster systems were accomplished in cooperation with the group of N. Rutsch from the Technical University (TU) of Munich, Germany, which has developed efficient parallel KF-based program ParaGauss [9]. On some zeolite-related problems, we have also collaborated with the groups of V. Nasluzov from the Institute of Chemistry and Chemical Technology (ICCT), in Krasnoyarsk, Russia, J. A. Lercher from the Technical University of Munich, Germany; and B.C. Gates from the University of California, Kaysville, USA. We also work with three Bulgarian groups, that of K. Hadjiivanov from the Institute of General and Inorganic Chemistry (IGIC) of the Bulgarian Academy of Sciences (BAS), Sofia, leading in the experimental IR characterization of zeolites with probe molecules, that of A. Bojilova from the Faculty of Chemistry of the University of Sofia, an expert in the synthesis and reactivity of coumarin and phosphonocoumarin derivatives, as well as with the theoretical group of T. Mineva from the Institute of Catalysis (IC) of BAS, with whom we share common interests in various studied systems and computational approaches. A crucial factor for a successful research and international cooperation is the reliable funding of the research activities and here I would like to thank the Bulgarian National Science Fund for the financial support under the National Research Program *Nanotechnologies and New Materials*. This new generation of research funding programs of the Bulgarian Ministry of Education and Science is very useful for acceleration of modern research in this country since it is oriented towards the hottest scientific and technological areas and allows cooperation between several research groups, creating the basis necessary for innovative multidisciplinary research. The new programs for specific support of research activities in the uni-

versities and career development of junior scientists are also quite timely and we hope that these encouraging initiatives for strengthening of the national research potential will be further extended with programs for innovation and improvement of the research equipment and infrastructure. We are also grateful to the Alexander von Humboldt Foundation and the Deutsche Forschungsgemeinschaft, Germany, that have supported our joint research with the group of N. Rösch.

First, I will summarize our works on understanding the properties of extra-framework metal cations in zeolites. Such cations can be included in zeolites during the synthesis or *via* post-synthetic exchange and typically occupy defined positions in zeolite cavities (Fig. 2) in the vicinity of Al centers in the framework due to the excess of negative charge at the oxygen centers around them [10]. Particular interest in these charge-compensating metal cations is connected, on the one hand, with their influence on the zeolite framework properties, such as acidity of neighboring κ H groups and basicity of the oxygen centers from the framework. In this way, by cation exchange, one could control to some extent these important properties of the material. On the other hand, the exchanged metal cations, particularly of transition metals, feature a peculiar catalytic activity and selectivity, which often cannot be achieved by non-exchanged forms of the zeolite catalysts. For this reason, we studied the location and sorption properties of a series of alkaline [11,12], alkaline-earth [13] and some transition metal cations [14, 15, 16]. We have shown that smaller alkaline and alkaline-earth cations, Li^+ , Na^+ , Mg^{2+} , Ca^{2+} , are located at the six-membered ring in faujasite (FAU) type zeolites but their exact location with respect to the framework depends not only on the corresponding ionic radius but also on the number of Al atoms in the zeolite ring.

All cations of alkaline, alkaline-earth and transition metals interact stronger with the zeolite oxygen centers bound to the Al atom from the framework. For this reason, we investigated the properties of these κ centers and found that they are characterized by a higher basicity compared to other κ centers in the zeolites, as evaluated by the calculated proton affinity (PA) of

oxygen atoms [17]. In order to facilitate the experimental determination of the zeolite basicity, we tried to establish a connection between the PA and experimentally measurable quantities that would allow the construction of a general scale of the basicity of zeolite oxygen centers. For this purpose, we first investigated the shifts $\Delta E_b(\kappa 1s)$ of the 1s core level of these oxygen centers that could be measured by X-ray photoelectron spectroscopy (XPS) [17]. The PA values of oxygen atoms in the studied models and their calculated core level shifts $\Delta E_b(\kappa 1s)$ were found to correlate very well. From the slope of this high quality correlation line we conclude that a negative shift of the $\kappa 1s$ binding energy by 1 eV (due to destabilization of the $\kappa 1s$ level) implies an increase of the PA by 82 kJ mol^{-1} . Such a linear correlation has been observed experimentally for the PA and $E_b(1s)$ values of a series of oxygen- and nitrogen-containing molecules in the gas phase [18]. The second characteristic feature, which we checked, was the shift of the IR frequency of the κ H group of a probe molecule, which forms a hydrogen bond with the basic site, namely methanol [19, 20]. The shifts of both stretching and deformation κ -H vibrational frequencies of methanol adsorbed on alkali-exchanged zeolites were found to correlate with their calculated PA. After additional calibration of the calculated PA values and comparison with the *measured* IR frequency shifts [21] of adsorbed methanol we derived two simple equations allowing experimental determination of the PA values of zeolite oxygen centers using the IR spectra of adsorbed methanol. Specific advantage of this approach is the "experimental" determination of the PA value of a particular type of oxygen centers using simultaneously two different experimental numbers, the shifts of κ -H stretching and deformation bands, thus offering a reduction of the error from the measured frequencies. In agreement with the experiment, our calculations suggested that the proton affinity of oxygen centers in the K^+ form of the zeolite model are by 23-29 kJ/mol higher than those of the corresponding Na^+ model. As an estimate, the most basic κ centers in the Na^+ form of FAU zeolite were found to have PA similar to that of ammonia, 885 kJ/mol, while the PA of the oxygen centers in the Al-free zeolites is calculated

to be close to that of water.

While alkaline and alkaline-earth cations exist as bare species coordinated to the basic centers of the zeolite framework, the experimental establishment of the actual chemical form of various other metal cations is often ambiguous. For instance, cationic zinc species in zeolites could exist in several forms: Zn^{2+} , ZnKH^+ , $[\text{Zn}-\kappa-\text{Zn}]^{2+}$, or $\text{Zn}(\text{H}_2\kappa)^{2+}$. The zeolites containing cationic zinc species show much higher activity in the catalytic dehydrogenation of alkanes to alkenes and aromatics, as compared to the zinc-free form of HZSM-5 zeolite [22]. Our recent computational modeling [16] of these species located in the channels of ZSM-5 zeolite has shown that the most stable form is $\text{Zn}(\text{H}_2\kappa)^{2+}$, suggesting a rather high desorption energy of water in the complex, 130-184 kJ/mol, depending on the position of the Zn^{2+} cation with respect to zeolite wall. In addition to this energetic argument, the obtained location of the $\text{Zn}(\text{H}_2\kappa)^{2+}$ species and the corresponding interatomic distances fit to the available experimental EXAFS data [22]. Since these calculations were based on an isolated fragment of the zeolite, we are currently investigating the influence of the rest of the zeolite framework on the state of zinc species, employing the advanced hybrid approach *covEPE* for modeling of zeolite structure (see below) [23, 24]. Using the obtained structures of the four different zinc species, we are also working on the derivation of some experimentally observable characteristics, such as κH frequency, in species where such groups exist, and IR frequencies of adsorbed molecules, more particularly H_2 . For this reason, we are now simulating molecular sorption and dissociation of H_2 on the four types of cationic Zn species that will facilitate the assignment of the experimentally observed species or, at least, will allow formulation of criteria for such discrimination in future experiments. In addition, upon comparison of the relative stability of adsorbed H_2 , we will make clear which cationic Zn species are expected to be most reactive in dissociating H_2 and which would facilitate the recombination to molecular hydrogen, the latter being assumed as the rate-determining step [22] in ethane dehydrogenation.

In various cases, crystallographic studies do not provide reliable information about the posi-

tions of the exchanged metal cations, and sometimes this information is even misleading [11]. In such cases, substantial experimental information can be obtained from the IR spectra of adsorbed probe molecules, particularly $\text{C}\kappa$. As it was recently reviewed [7], this approach provides direct information on the coordination vacancies of the cations, hints for their location and mobility in zeolite channels, as well as their reactivity. In this respect, our computational modeling suggested that the frequency shift of $\text{C}\kappa$ adsorbed on Na^+ cations in zeolites depends on the number of Al atoms in the neighboring zeolite ring. We also made an important contribution to the elucidation of the structure of the cationic rhodium dicarbonyl complex embedded in the cavities of dealuminated Y zeolite (KAY). This material is characterized by two very sharp IR bands of $\text{C}\kappa$ symmetric and antisymmetric modes confirming the formation of dicarbonyls and implying uniform location and structure of the $\text{Rh}(\text{C}\kappa)_2^+$ species. However, the combination of experimental IR and EXAFS data does not lead to direct determination of the location and structure of the complex in zeolite cavities. With the help of a series of KF model calculations [14], we were able to identify the adsorption complex (Fig. 3) that fits best the experimental characteristics obtained by EXAFS and IR spectroscopy. Excellent correspondence between the calculated and experimental frequency shifts of the $\text{C}\kappa$ ligands in the complex encouraged us to address a more complicated problem, i.e., the assignment of an experimental band at 2093 cm^{-1} assumed to correspond to $\text{Rh}(\text{C}\kappa)^+$ [25]. Our simulations, however, suggested that this band should be assigned to rhodium carbonyl species, which contain additional hydrogen ligands, e.g., $\text{Rh}(\text{C}\kappa)(\text{H}_2)^+$ or $\text{Rh}(\text{C}\kappa)(\text{H})_2^+$, whereas the zeolite-supported complex $\text{Rh}(\text{C}\kappa)^+$ is characterized by the IR band observed at 2014 cm^{-1} .

The presence of metal cations in zeolite pores determines in various cases their sorption properties and can be used for the stable immobilization of sorbed organic molecules in zeolites (Fig. 4a). Our recent calculations [26] on the formation of a chelate complex of phosphonocoumarin derivatives suggested that such a complex is rather stable, even with a cation as Na^+ (Fig. 4b), which is not a typical complex-

forming cation. However, when complexes with neutral ligands are modeled, one should include not only a bare cation, but also a species representing the counter-anion in order to obtain reliable values for the complex formation energy and the correct structure of the complex. Otherwise, the complex formation energy would be considerably overestimated. These calculations also allowed elucidation of the experimentally observed complete regioselectivity for acylation of the diethylphosphonocoumarin. The detailed electron density distribution and bonding analysis in this study, based on the natural bond orbital analysis (NBK) [27], has shown a particularly high negative charge, -0.59 e (and a respective higher reactivity) of the carbon atom, which is connected with strongly positively charged centers, phosphonic P and lacton C atoms, and also participates in a double C=C bond.

Another substantial part of our research is directed to modeling of metal clusters supported in zeolite cavities. Supported metal clusters play an important role in nanoscience and nanotechnology [28] with a variety of applications in advanced heterogeneous and environmental catalysis, microelectronics, magnetic recording, etc. A typical application is in the automotive catalysts for reducing the car exhaust that contain supported small particles of palladium, platinum, and rhodium. Other applications of importance in chemical industry are transformations of alkanes and alkenes on transition metal clusters in zeolites. Specific application of supported metal clusters is related to production of chemical sensors, capable of detecting the presence of molecules in the atmosphere by means of their reaction with the supported metal particle.

Typically in these applications, the efficiency and often the activity of the material increases with the decrease of the cluster size. For this reason, zeolites are very suitable as supports (hosts) of such metal particles since the dimensions of their cavities in nanometer and sub-nanometer scale are strictly limited by the crystallographic structure that allows an efficient control of the size of metal particles embedded inside the zeolite. These strict spatial limitations allow preparation of uniform encapsulated metal moieties, which is crucial for the selectivity in further cata-

lytic applications of the material. Precise control of the size and uniformity of the metal clusters is much more complicated on "open" surfaces. This advantage of the zeolite-supported metal clusters stimulated us to study their structure and bonding to the host framework. In particular, we considered encapsulated transition metal clusters because of their industrial importance and because precise experimental information is available for some of these systems [29, 30]. The measurements suggest the clusters with defined nuclearity, 4 or 6 metal atoms, in zeolite cages.

We studied most extensively Rh_6 clusters embedded in FAU zeolite [31, 32] since such species have been experimentally investigated by Gates and co-workers [29] with EXAFS, which provided estimates for the local coordination and interatomic distances of the Rh atoms in the cluster. The experimental distances were, however, notably longer than the values obtained by density functional modeling for non-reactive adsorption of the bare Rh_6 cluster (Fig. 5a), which could not be explained simply by standard errors from the experimental fit of the computational method. In order to solve this problem, we simulated various investigated structures of the cluster, accounting also for the possible presence of impurity atoms in the system, namely H, C, and K [32]. Model clusters with C or K impurity atoms were not considered pertinent due to deviations from the experimental findings. However, a structure of the Rh_6 cluster covered additionally by three H atoms (Fig. 5b) was found to agree closely with the EXAFS interatomic distances, while for all other structures such an agreement was not observed. The modeling suggested that these H atoms originate from the neighboring KH groups of the zeolite and undergo reverse spillover onto the metal cluster. This process is accompanied by a partial oxidation of the Rh atoms bound to the zeolite cluster. In addition, the quantum chemical modeling yielded a notably higher stability of the "reactive" structure of the Rh_6 cluster covered by H atoms, as compared to the non-reactive case. However, it remained unclear whether this reactivity of supported Rh_6 clusters with KH groups of the support is a peculiarity inherent to rhodium or whether such a phenomenon can occur also with other subnano-size clus-

ters of transition metal atoms. In order to answer this question, we are currently modeling non-reactive and reactive adsorption of hexaatomic clusters of 3d, 4d, and 5d transition metals from Groups 8-11 of the Periodic System, which are most important for catalytic applications. For these calculations, we used the same method and zeolite model as for the embedded Rh_6 cluster (Fig. 5). Just as for Rh_6 , we found that the reverse hydrogen spillover (Fig. 6) from hydroxyl groups of the zeolite is energetically strongly preferred for most elements of Groups 8–11, by at least 90 kJ/mol per proton. For Ag_6 and Au_6 , however, this energy is much lower. Thus, as concluded earlier for Rh [31], it does not seem possible to prepare bare metal clusters of Groups 8–11 in zeolite cavities or on a hydroxylated oxide surface.

In order to better understand the interaction of the transition metal cluster with the support, we studied isolated metal clusters, often called “gas phase” clusters. Using these models, we first checked the influence of the impurity atoms on the cluster magnetism and structure, on the examples of Rh_6 and Ni_4 clusters. The location of the H, C, and κ atoms inside the cluster was found disfavored, compared to the outside location, even for the larger Rh_6 cluster. In all studied cases, we found a considerable stabilization of all electronic levels in the ligated clusters and a partial rearrangement of the electron occupation on frontier d and s orbitals of the metal atoms (Fig. 7). For instance, for a Ni_4 cluster with C impurity only, this rearrangement is strong enough to quench the spin multiplicity of the cluster by a factor of 2 [33].

In addition to the binding of an impurity atom on the metal cluster, we investigated the coordination of diatomic molecules [34]. As an example, the exhaustive study of various coordination structures of 1 to 12 dinitrogen molecules to a Ni_3 cluster can be mentioned. Although the N_2 molecule is rather inert, we found that in the most stable structures it is bound by more than 110 kJ/mol per ligand, which expands the Ni-Ni bonds. The preferred way of bonding of the ligand is the linear coordination to a Ni atom (Fig. 8a), but in some structures simultaneous coordination to the three Ni atoms of the cluster is also rather stable (Fig. 8b). With the increase of the number of N_2

ligands coordinated to the cluster, we found an expansion of the metal cluster (Fig. 8c). Using the obtained energies of binding of the ligands to the Ni_3 cluster, we were able to simulate the evolution of different types of $\text{Ni}_3(\text{N}_2)_x$ species with an N_2 partial pressure that predicted destruction of the cluster into mononuclear species for $\text{N}_2:\text{Ni}_3$ ratios above 7.

In addition to the investigation of the structure and chemical features of different types of catalytic systems or composite materials, we have participated in the development of a new hybrid quantum mechanical/molecular mechanical (QM/MM) approach *covEPE* (Elastic Polarizable Environment for materials with covalent polar bonds) [23, 24]. With such hybrid approaches, one can model extended and complex systems employing high level computational methods for the chemically relevant part of the system (e.g., active site, metal cluster, etc.) and include explicitly the rest of the system at a more computationally economic level, typically at molecular mechanics. The main advantage of these combined methods over the isolated cluster models is the relevant accounting for the long-range electrostatic effects of the environment and the short-range constraints of the neighboring centers. However, the construction of a QM/MM scheme is not trivial; various complications related to the QM/MM interface, the coherence in the description of the modeled system by the used QM and MM methods, etc., should be taken into account. We turned towards the development of a new embedding approach for zeolites and covalent oxides since the available hybrid schemes had some drawbacks, such as introduction of “artificial” atoms on the QM/MM border or utilization of too large charges [35]. From the very beginning, our scheme [23] was designed to avoid these (and also other previous) deficiencies by the construction of a special type of border atoms and parameterization of a new force field for zeolites that employs realistic potential-derived charges. In addition, we applied special scheme providing self-consistency of the embedding, developed previously within the version of the EPE method for ionic oxides [36]. The performance of the method was checked for three zeolite structures with different composition and simulated structural parameters, vibrational

frequencies, and acidity of the zeolite materials were found to fit well to the experimentally measured characteristics. Due to the complexity of the problem, this method was developed in cooperation with the groups of N. Rüsç (TU Munich) and V. Nasluzov (ICCT, Krasnoyarsk). As a result of these joint efforts, now we benefit from the most consistent and reliable hybrid QM/MM scheme for zeolites and covalent oxides. Using this approach, we recently found that the location of the acidic KH groups in zeolites and the framework structure affect their properties stronger than the Al content of the zeolite [24]. In addition, now we can evaluate the contribution of the distant zeolite framework to the calculated characteristics by comparing the results from isolated and embedded cluster models. This contribution is actually a partial estimate of the error of the isolated cluster calculations for the considered system. Such calculations were performed in our study of the type of cationic Zn species in ZSM-5 zeolite, mentioned above [16]. Due to proper accounting of the relaxation of the zeolite framework in *covEPE*, all types of modeled Zn species were bound more stably in the embedded cluster model, particularly the Zn^{2+} cation with a difference in the binding energies of more than 70 kJ/mol. Currently, we are employing the *covEPE* method for other important materials, zeolites containing transition metals in framework positions as titanium silicalite, and subnanosized metal clusters sorbed inside zeolite cavities.

I do hope that this brief review exemplified the orientation of research groups in Bulgaria towards the modern fields of science and technology and the advanced approaches for their exploration. In the spirit of contemporary international research, we are working in cooperation on both national and international levels, expecting successful joint achievements. Particular efforts are lately focused on the increase of participation of Bulgarian research groups in the European research area in the frame of the 6th Framework program, although the very tight competition in FP6 discourages many good teams in this country. We have also restored the organization of scientific meetings and conferences, which is another important part of the national and international collaboration. In recent years, owing to the

support of the Stability Pact for South Eastern Europe, several international conferences were organized in Bulgaria. Our group together with T. Mineva (IC, BAS) initiated and organized two Humboldt Conferences on Computational Chemistry in 2002 and 2004 that promoted both the regional cooperation in the field and strengthened our connections with scientists from other parts of Europe. We also organized two bilateral German-Bulgarian workshops in 2003 and 2005, in cooperation with K. Hadjivanov (IGIC, BAS), and with the support of the A. von Humboldt Foundation. Here, I should also mention the generous support for the organization of the internal seminars provided by the National Science Fund within the program *Nanotechnologies and New Materials*. Accounting for the importance of the training and communication skills of students and junior scientists in their further career development, since 2001 we have carried out annual Scientific Sessions for Undergraduate and Koctoral Students in Chemistry with the assistance of the Humboldt Union in Bulgaria, the Faculty of Chemistry, the Students' Council, and the "Evrika" Foundation. During these events, the participants not only presented their research results, but also got in touch with the latest achievements of the leading scientists in Bulgaria, such as Academician P. Bontchev, Acad. E. Golovinski and Prof. B. Toshev. The constantly growing number of participants in these national sessions has clearly shown the keen interest of the new generation of scientists in the advances in modern chemistry.

Finally, I would like to express my gratitude to the National Center for Information and Documentation for offering me this special opportunity to present our recent research efforts as an example of the current research activities in Bulgaria.

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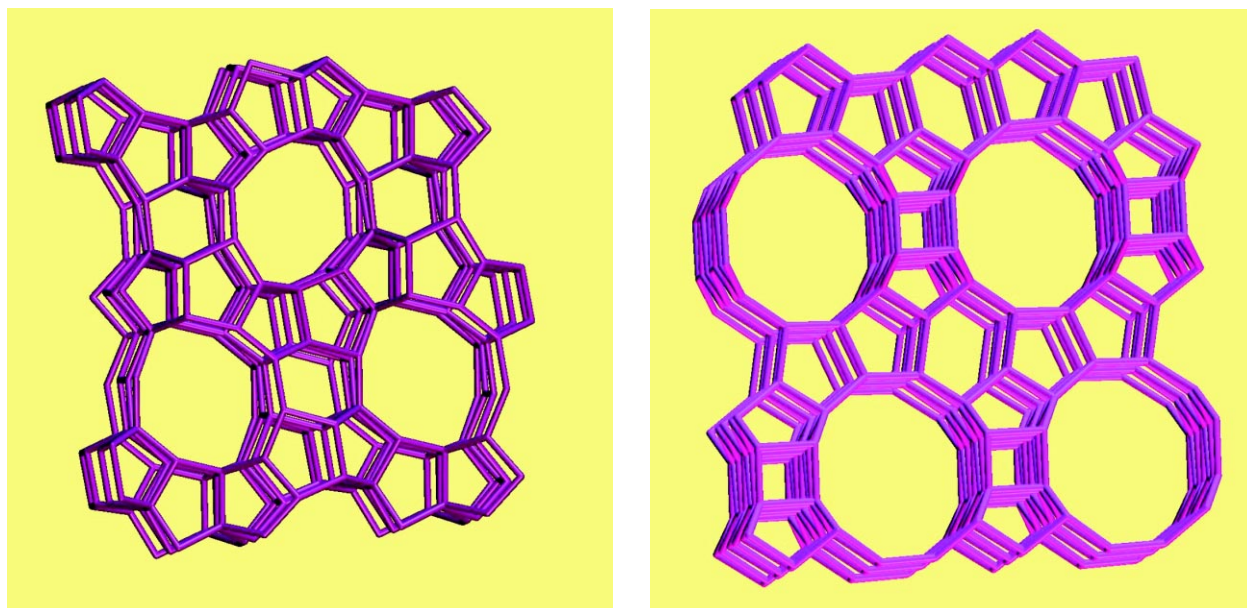


Figure 1. Framework structures of MFI (a) and BEA (b) zeolites.

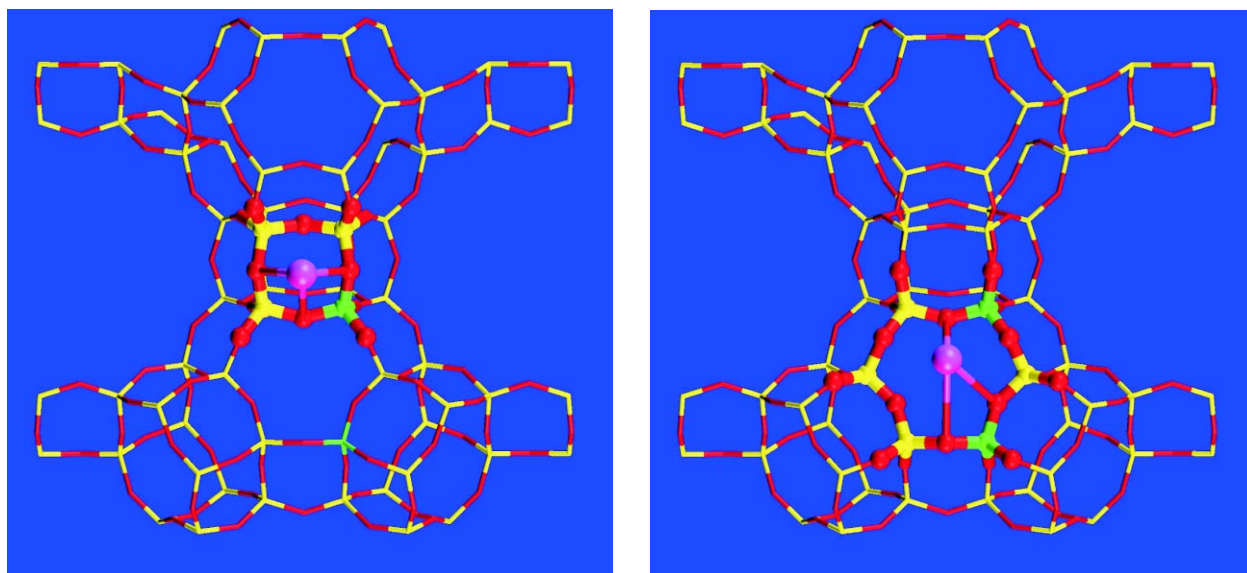


Figure 2. Sketch of the cationic positions at four-membered (a) and six-membered (b) rings of FAU zeolite framework. Atoms participating in the fragment of the zeolite framework used in computational modeling are shown as balls.

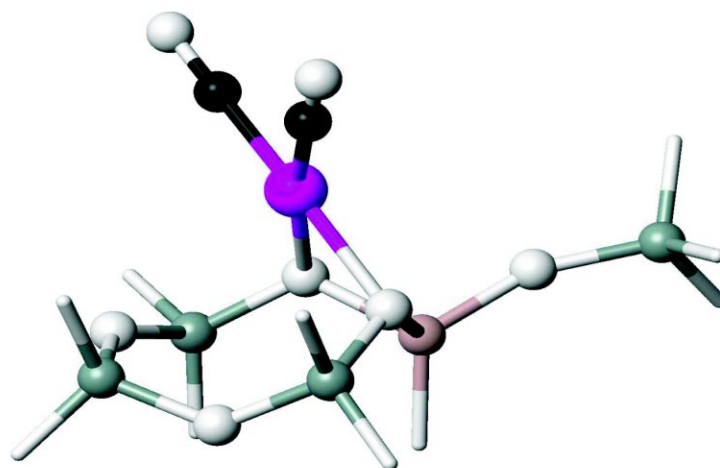


Figure 3. Structure and location of $\text{Rh}(\text{C}\kappa)_2^+$ complex in dealuminated Y zeolite determined by KF modeling and comparison with experimental spectra.

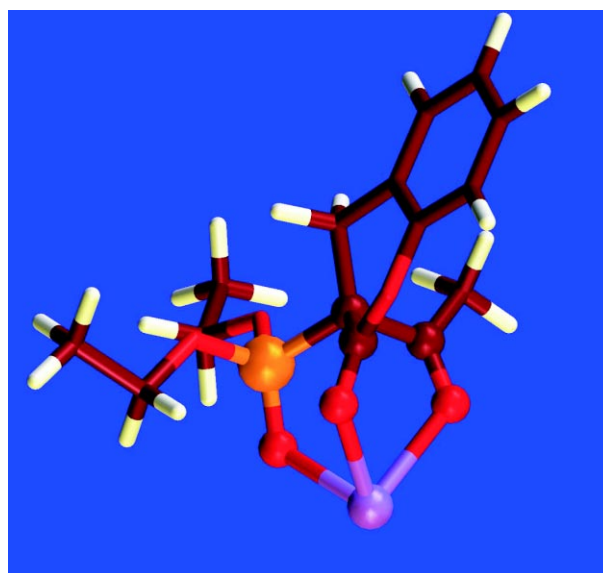
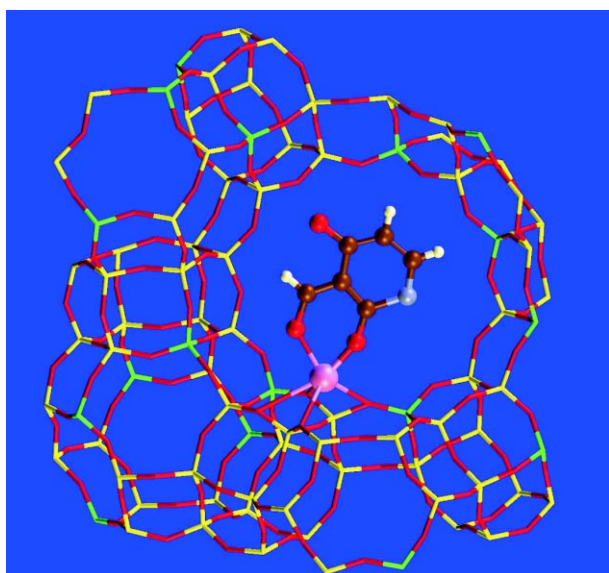


Figure 4. Sketch for the immobilization of the organic compound in zeolite cavity by formation of chelate complex with extraframework metal cation (a). Corresponding model calculations are performed with larger phosphonocoumarine molecule and isolated (b) or coordinated to acetate anion cation.

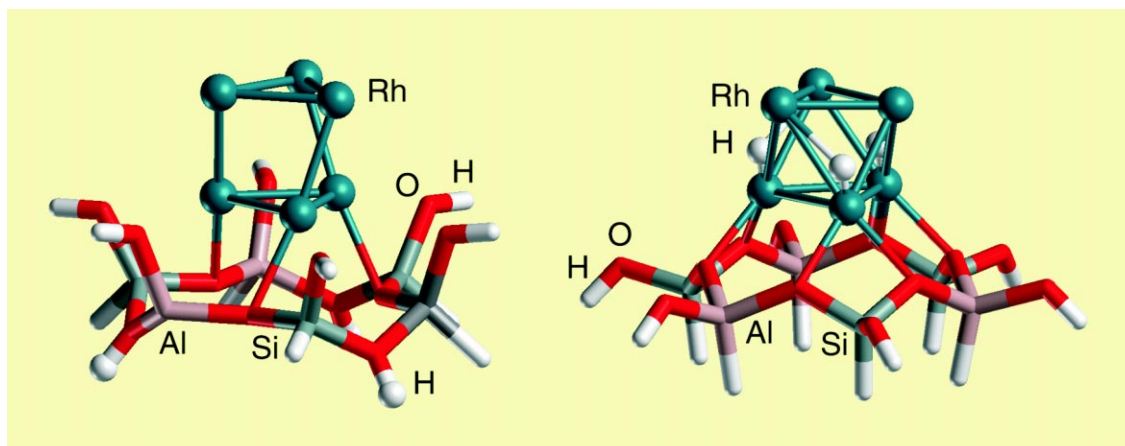


Figure 5. Structure of Rh_6 cluster embedded in Y zeolite without migration of the protons from the zeolite KH groups (a) and after migration of the protons onto the metal cluster (b).

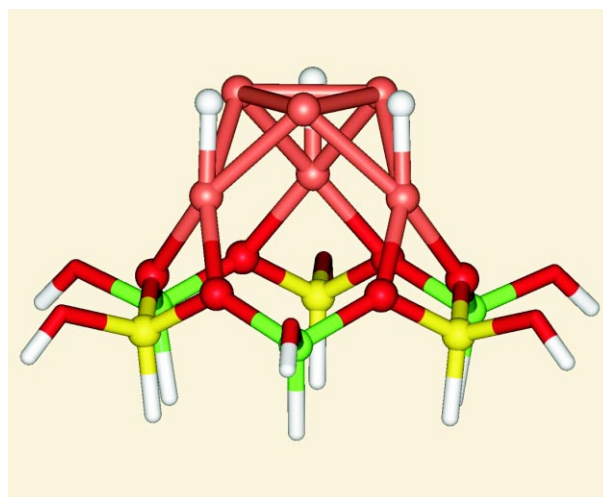
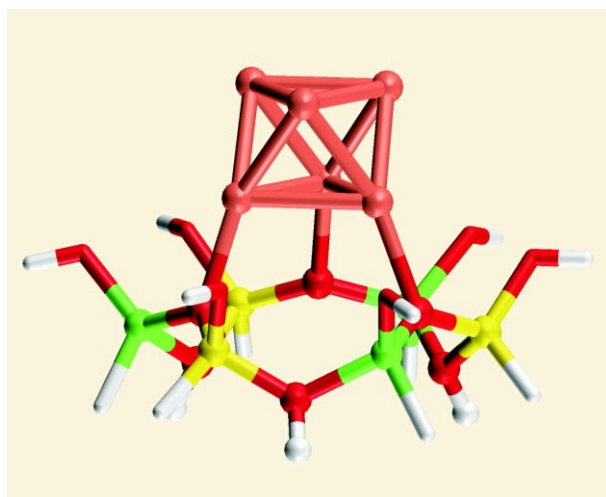


Figure 6. Structure of Cu_6 cluster embedded in Y zeolite without migration of the protons from the zeolite KH groups (a) and after migration of the protons onto the metal cluster (b).

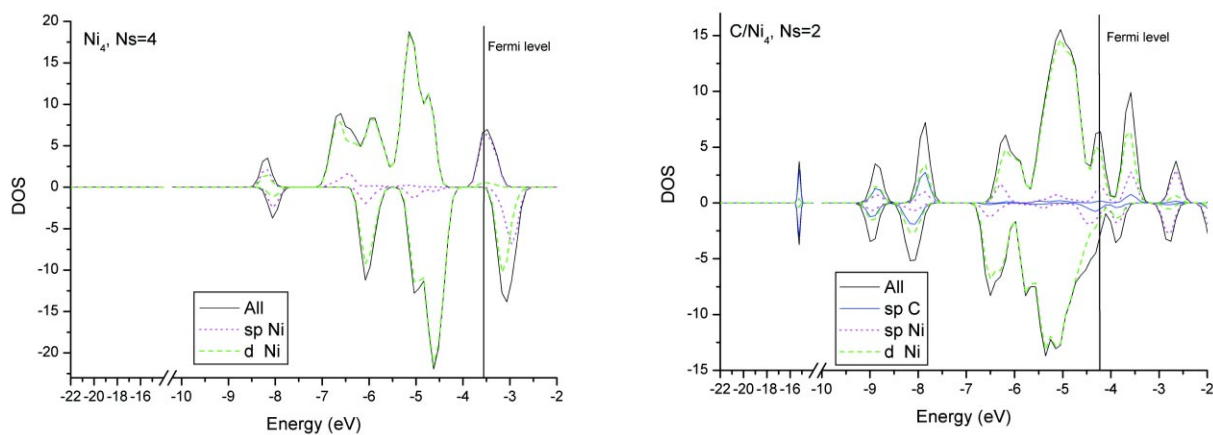


Figure 7. Density of states (DOS) plot for Ni_4 (a) and Ni_4C (b) clusters. The contributions of the frontier s and d orbitals of Ni atoms are shown in red and blue, respectively.

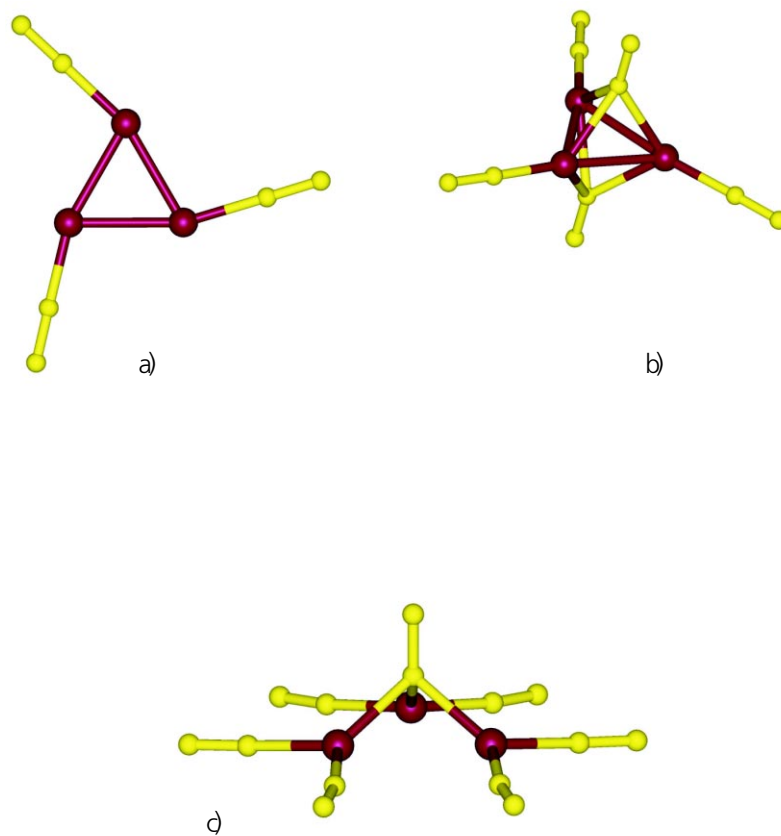


Figure 8. Optimized structures of Ni_3 cluster with 3 (a), 5 (b) and 7 (c) N_2 ligand molecules.



BULGARIAN ADDED VALUE TO ERA

ABI - AGROBIOINSTITUTE - CENTRE OF EXCELLENCE IN PLANT BIOTECHNOLOGY

Address: 8, Kragan Tsankov Blvd., 1164 Sofia, BULGARIA, Tel.: +359 2 963 54 07,
Fax: +359 2 963 54 08, E-mail: atanas_atanassov@abi.bg

AGROBIOINSTITUTE (ABI) is an independent state administrative institution formed under the supervision of National Center of Agricultural Sciences (NCAS), under the Ministry of Agriculture and Forestry. It was formed in 2000 as a result of reorganization in NCAS and incorporation of the Institute of Floriculture, Negovan and the Central Experimental Station, Samokov with the Institute of Genetic Engineering (IGE).

Under the new system ABI is trying to conduct flexible research programs with the mission of promoting the development of sustainable agriculture and forestry compatible with the environmental preservation but not ignoring the opportunities that the modern plant biotechnology offers.

MILESTONES

- Since 1995 ABI represents Bulgaria at the International Centre of Genetic Engineering and Biotechnology (I.C.G.E.B.), Trieste, Italy.
- Since 1995 former IGE (ABI) is a member of Norman Borlaug Institute for Plant Research at the Ke Montfort University (KMU), Leicester, UK, together with institutes and universities from UK, Czech Republic and China.
- In 1999 the Institute was selected as a Centre of Excellence in the frames of INCK 2, FP5 EC Program, responsible for co-ordination of scientific investigations and training in the field of plant biotechnology on the national and regional level.
- Since 2000 ABI is a member of Euro-

pean Plant Science organization (EPSK).

- Since 2002 ABI is a member of European Federation of Biotechnology (EFB).
- In 2002 ABI was selected as a sub-regional centre for Eastern Europe in the field of regulations and control of GMK.

MANAGEMENT

Director:

Prof. Atanas Ivanov Atanassov

(Prof. Kr. Sci., Member of Bulgarian Academy of Sciences, Member of Agricultural Academy of the Ukraine, Member of Agricultural Academy of Russia, Koctor Honoris Causa of Agricultural University and Veterinary Medicine, Kluj-Napoca, Romania)

Address:

8, Kragan Tsankov" Blvd.,
1164 Sofia
BULGARIA
Phone: +359 2 963 54 07
Fax: +359 2 963 54 08
Mobile 0888714154
E-mail: atanas_atanassov@abi.bg

AGROBIOINSTITUTE is the only research institute in the country, whose activities are governed by the International Consultative Council (ICC) (VIII-th ICC will take place on October 1–2, 2005). Leading world-recognized scientists in the field of plant biotechnology are included. Members of the National Council of ABI are also

included in the staff of the ICC. According to the decision of the First meeting of ICC in 1988 and the scientific policy of the Institute, guests (national and international) may take part in the meetings, too.

RESOURCES

In March 2003 AgroBioInstitute (ABI) moved from Kostinbrod to Sofia. Now, experimental work is carried out in the new premises of AgroBioTech Park (joint initiative between ABI and Faculty of Biology, Sofia University "St. Kl. khridski").

There is complete and rather new modern biotech equipment for *in vitro* culturing and analysis in ABI – Keparment Sofia. Research and technical staff is trained in leading foreign plant biotech laboratories and successfully uses modern methods and technologies for the main crop species: (i) *in vitro* regeneration; (ii) gene cloning and transfer; (iii) molecular markers; (iv) analysis of transgenic plants; (v) techniques and methods for clonal micropropagation and diagnosis, etc.

Tissue Culture Lab near Negovan is built in 1986 both to establish new technologies for micropropagation of virus free planting material and to develop protocols for regeneration and clonal micropropagation of different ornamental species. There are arable lands to produce ornamentals and potatoes in other two departments.

Total staff of ABI numbers 97 persons. The research staff is a multidisciplinary team of 42 well-trained specialists: 20 – senior researchers and 22 – researchers. 162 specializations in 20 countries are realized during 1985 – 2003. The institute is accredited to teach PhK students on GENETICS, PLANT PRkTECTIkN and kRNAMENTAL PLANTS. At present there are 23 PhK students in ABI.

The list of current (2005) projects of AGRkBIkINSTITUTE includes:

National funds:

- National Center of Agricultural Sciences
 - 23 projects
- National Council "Scientific Investigations"
 - 9 projects

International funds:

- Bilateral cooperation 12 projects
(Belgium, China, Greece, Japan, Turkey, Vietnam)
- GEF/UNEP 1 project
- NATk 2 projects
- EC FP 5 6 projects
(three of them already finished)
- EC FP 6 4 projects
- CkST Actions 9 projects

Annual budget of ABI during the recent three years is about 800 000 EURk.

The structure of ABI is very flexible. Working groups are the main research structural units. At present there are 14 working groups. Research topics are as under:

A. Kevelopment of systems for direct and indirect *in vitro* regeneration and somatic embryogenesis of economically important crops (diploid and tetraploid *Medicago* sp., cereals, vegetables (tomato, pepper, etc.), *Vitis* sp., ornamental and oil rose, small fruits, herbs, flax, medicinal and ornamental plants) - molecular and cellular aspects.

B. Engineering of abiotic (drought, temperature, heavy metals, herbicides etc.) and biotic (disease', parasitic plants, etc.) stress resistance in model (tobacco) and various crop plants (barley, wheat, maize). Parasitic plant management in sustainable agriculture. Kevelopment of systems for fast screening and evaluation for stress response. Genomic studies of model stress tolerant plants.

C. Genetic transformation (direct and indirect gene transfer) for crop improvement: (i) tetraploid alfalfa, wheat, barley, maize, etc. – for food and feed quality; (ii) production of therapeutic proteins (hLF) (in barley and tetraploid alfalfa); (iii) fiber quality – in flax; (iv); rose, carnation and *Antirrhinum majus* - for improvement of ornamental traits.

D. Kevelopment and application of SSR and TK markers in *Vitis* sp., *Rose* sp., small fruits, barley, wheat and maize for variety identification and MAS for food and feed quality improvement and abiotic stress factors.

E. Evaluation of the quality (protein, fat, fibers, ash and moisture content) of crops and agricultural products and development of spe-

cific calibration models for NIRS detection of genetically modified plant material (GMk) by Near Infrared Spectroscopie (NIRS analysis)

F. Good agricultural practices for optimizing of variety trials in conformity with the EC-directives and reduction of soil erosion by "reduced-tillage" cultivation technique.

G. Gene bank of vegetatively propagated species (*Vitis* sp., ornamental and oil rose, small fruits, herbs). Identification & Detection of Virus Kiseases – by grafting and serological analyses (ELISA), KNA identification, somaclonal variation, clonal micropropagation and long-term in vitro storage in low temperatures.

H. Development and adoption of strategic documents on biosafety (GMk laws). Development of a system for handling requests for permits for certain activities with GMks, as contained use, releases into the environment and placing on the market. The system provides for administrative handling, risk assessment, decision-making and public participation. Development of systems for enforcement and monitoring, public information and public participation, i.e. systems for providing information to stakeholders and involve them in the development and implementation of the national biosafety framework. Development of national biosafety database

I. Participation of the Bulgarian Biotechnology Information Center (Bg BIC), as a pilot initiative within the frame of Global Knowledge Center on Plant Biotechnology, in the International Service for the Acquisition of Agri-biotech Applications (ISAAA, www.isaaa.org). BgBIC is a part of a global network of 13 similar centers spread on four continents: Asia, Africa, Latin America and Europe. The AgroBioTech Park (ABTP) – a joint initiative between the AgroBio-Institute (National Center of Agricultural Sciences) and the Faculty of Biology (Sofia University) host BgBIC. ABTP was officially opened in 2003.

AgroBioInstitute was able to come to part of our efforts on the official establishment and operation of Accredited laboratory in regard to the evaluation and testing of phytosanitary status, genetic authenticity, KNA detection and forage quality of plants. It will definitely strengthen

practical contribution of ABI to the Bulgarian agriculture especially for the farmers and entrepreneurs.

For several years the Institute is coordinating the activities related to the development and implementation of the **National biosafety framework for utilization of genetically modified organisms (GMO)**. For its activities and initiatives in the area of Biosafety in 1999 ABI was selected as a **Sub-regional Centre for Eastern Europe** in the field of regulations and control of GMk.

Alliances/Partners Sought:

ABI dedicates its work to multidisciplinary research, combining the traditional biological and breeding approaches with techniques relevant to functional genomics, looking for biological process by which we can design better crops with higher-yield, low-impact agriculture, but also to the development of novel products valuable for their food quality and friendly to human health and environment. The institute is looking for partners for joint venture projects, product development and scientific co-operation and exchange that will further support the main scientific and scientifically applied priorities of the organization as:

- Creation of a **database bank for the available biodiversity of collections of plant resources, forms and plant lines**; molecular-genetic assessment of their suitability for including into the selection process as well as their use in practice;
- Creation of a **database bank for the available varieties, hybrids and animal breeds**; assessment of their commercial value and possibility for their genetic improvement; creation of molecular marker systems for the purpose of effective realization in practice of the plant varieties and animal breeds with high productive potential;
- Creation of **seed and planting material** from local and introduced sorts and hybrid plants, appropriate for the purposes of the alternative and/or organic agriculture;
- Creation of technologies for effective manufacturing of biological (ecological) products and safe foods; analysis and assessment of the ex-

isting **methods for biosafety and control** regarding their timely use in the systems of organic and intensive agriculture;

- Use of biotech methods connected with microclonal propagation, **analysis of the plant health and genetic status** with the purpose of improving the existing technologies for accelerated **creation of quality base and super elite seed and planting material** from economically important agricultural crops and herbs.

- Creation of a **working system for cooperation between scientific-applied laboratories and final consumers** of seed and planting material;

- Kevelopment and applying of contemporary approaches based on KNA molecular markers, **improving effectiveness of the breeding process, saving and keeping the purity and**

quality of the seed and planting material for agricultural crops, assessment of the existing but not used at the moment genetic diversity of wild and/or crop ecotypes. The aim is for them to be included in the genome programs and/or to be used directly for selection of plant varieties suitable for alternative agriculture;

- Keveloping and/or adapting of **effective systems for genetic cloning and genetic transfer** necessary for the genetic–breeding programs for plants and animals;

- Creation of **data bank of the available genetic resources in animal breeding** and especially of the becoming extinct and threatened with extinction native animals.

- Keveloping **systems for restoring the threatened with extinction local populations** due to small volume.



MADE IN BULGARIA WITH EUROPEAN SUPPORT

Use of Organogenic-mineral Sediments from the Bottom of the Black Sea as Ameliorant and for Other Aims

Prof. Petko Dimitrov

Institute of Oceanology, P.K. Box 152, 9000 Varna, BULGARIA

Area of application: *Agriculture*

Scientific teams from the Institute of Oceanology – BAS in Varna and Agriculture University in Plovdiv are working jointly on the problem of using deepwater organogenic-mineral deposits (sapropel, diatomitic and coccolithic oozes disposed at 500 to 2200 meters depth at the Black Sea bottom) as ameliorant for soils and substrates.

From 1997 to 2004 were carried out a series of experiments on different agricultures as wheat, tomatoes, pepper, eggplants, oleaginous rose and others.

Reasons for these joint research investigations give:

- The presence of inexhaustible reserves of alternative materials appropriate for improvement of soils;
- Eventual exploitation of these materials will not give negative consequences for marine environment;
- The existed technical base for their extraction for scientific and technological tests;
- The policy of European Union concerning agricultural needs, search for new alternative raw materials for improvement of the soil structure aiming ecologic agricultural production.
- The present-day condition of the soils in our country needs a new approach for their improvement and recultivation.

The ameliorant is applicable for reclaiming acid, microelement-poor and destroyed soils, as well as a substrate improver and also for recultivation of soils polluted with heavy and ra-

dioactive elements. It stimulates growth of plants, accelerates their ripening, increases yields, neutralizes soil acidity and increases their moisture absorption. The ameliorant is a deep-water Black Sea sapropel with the following composition, in %: Corg 3, Si₂ 3.13, Ca 14.5, Mg 2.75, Fe₂O₃ 4.57, Al₂O₃ 11.6, P₂O₅ 1.32, TiO₂ 0.4, chloroform extract 0.35, ethanoloacetone-benzene extract 1:1:1 0.30, Cu 0.03, Cr 0.0125, Mn 0.0365, Zn 0.0085, Mo 0.0175, Co 0.0155, Ni 0.0073, Li 0.0025, Sr 0.0061 and V 0.0088.

7 papers presenting the problem with the alternative raw materials used as ameliorant for soil and substrate improver were reported during the First International Workshop which was held from October 23rd to October 26th, 2004 in Varna, in the frames of European project within the 5th Framework (2003–2006) ASSEMBLAGE (Assessment of the Black Sea sedimentary system since the Last Glacial Extreme). These papers will be presented to the attention of EU experts in the beginning of 2005.

They are looking for possibilities for cooperation in the system of BAS, EU and private firms for introduction of the ameliorant in rural economy.

The patent for invention No. 63868 is issued on April 30, 2003 <http://www.bpo.bg/abstracts/pdf/2003/2003-04-p.pdf>.

Besides as an ameliorant for soils and substrates this alternative raw material can be used in ceramic industry, mud-cure, pharmacy and cosmetics as well as filters for purification of waters and gases, etc.

Using Natural Products Such as Pesticides and Growth-regulating Substances

Ass. Prof. Georgi T. Georgiev, MD, Academician M. Popov

Institute of Physiology of Plants, Acad. Georgi Bonchev Str., Bl. 21, 1113 Sofia, BULGARIA

Area of application: *Biologic farming*

The growing requirements to making food products in the recent years lead to the restriction of the synthetic pesticides application or to their full elimination in organic farming. Recently developed and proposed, the so-called Integrated Pest Management (IPM) programme aims at embracing the issue maximally by using different approaches. Biological pest-control including utilization of various allelochemicals – herbicides, insecticides, repellents, phytoalexins and fungicides, is the basic strategy in this programme. European legislation also focuses on the restriction of the use of synthetic chemical substances (fertilizers and pesticides) and stimulating the development of alternative methods for protecting and growing farming cultures (Council Regulation no. 2092/91; Law on Environmental Protection No. 137/1995). As an answer to these requirements the recent years in Bulgaria experienced the onset of the production of various preparations made from natural components. In answer to the pressing need of developing new technologies for the production and estimation of preparations applied in agriculture with a view to obtaining ecologically clean products, in the 1980s a team from the Institute of Physiology of Plants created new original technologies for obtaining and practical utilization of Lactofol leaf suspension fertilizers. The suspensions are a new generation of complex leaf fertilizers in which all the metal ions are bound to lactic acid that, after its assimilation by the plants, directly enters the metabolism and there are no remains of organic solvents in the production. Lactofol products have been registered by the Ministry of Agriculture and have been applied both in Bulgaria and in many other countries in the course of many years. Licensed so far are 8 modifications adapted in agriculture with a view to the availability of items, the specificity of the climate, the soils and the phase defi-

cits to different nutrition elements. Two new modifications are being developed at the moment. At the same time a team dealing with ethereal-oil and medical plants shaped up in the recent 10 years. The influence of various growth regulators for increasing the quantity and quality of ethereal oils is monitored, chemical activity of isolated oils and vegetable extracts, their impact on elimination of the harmful influence of some herbicides, as well as the growth-regulating and pesticide properties of these natural chemical substances are studied. As a result of these investigations, an agrotechnology was developed for influencing the growth and development of different types of wheat cultures as well as for carrying out pesticide control with the help of various plant extracts and ethereal oils from plants belonging to the families Labiatae, Compositae, Cupressaceae, Malvaceae and Umbelliferae.

Studying the impact of vegetable extracts from species belonging to the family Malvaceae on sprouts of plants (soya, beans, sunflower, maize and barley) treated with the Fluridon herbicide, Iliev et al. (Patent No 64220 B1/2004) established that the extracts eliminate the blocking effect of the herbicide on carotenoid biosynthesis ("bleaching" effect) and help the fast recovery of the damaged plants. In the different variants for establishing an allelopathic effect, elimination of the herbicide-induced changes after treating with vegetable extracts is observed. As early as after the very beginning of sprouting, up to the 2nd or 3rd leaf in monocotyledonous and up to the 1st or 2nd true leaf in dicotyledonous cultures, visible greening of the leaf mass occurs. Recorded in each of the following phases of development are: an increase of chlorophyll and soluble protein content in the leaves, of the intensity of $^{14}\text{CO}_2$ -fixation and of chlorophyll fluorescence. As a consequence of the allelopathic effect, stimulation of the growth of the

sprouts and the roots is also observed, as well as an increase of the fresh and dry weight of the vegetative mass. The use of biologically active substances of vegetable origin for protecting the cultural species of plants from the impact of

various phytotoxic factors is of major importance for the protection of the environment and especially for the development of organic farming, which is a priority in the common agricultural policy of the European Union.

Novel Nematode Lipid Binding Protein from *Ascaridia galli*

Associate Professor Ilia Bankov, DSc, PhD Rositsa Jordanova

Institute of Experimental Pathology and Parasitology
Akad. Georgi Bonchev Str., Bl. 25,1113 Sofia, BULGARIA

Area of application: Parasitology

The Institute of Experimental Pathology and Parasitology at the Bulgarian Academy of Sciences made a novel 55kDa LBP (Lipid Binding Protein) (ag50) (GenBank No AY587609) from the nematode *Ascaridia galli*. It was first identified as a LBP by its high binding affinity to [¹⁴C] palmitic acid. The partial amino acid sequence was obtained by direct N-terminal sequencing of the native protein, combined with protease digestion and sequencing of the internal peptides. Based on these data, primers could be designed and the full-length cDNA sequence was obtained. Sequence analysis revealed the presence of the signal peptide of 25 amino acid residues at the N-terminus and a conserved FAR (fatty acid and retinoid binding) domain at the C-terminus.

Ag50 revealed no significant homologies to other described LBPs. That is why it proposed ag50 as a novel parasitic LBP class. The wide occurrence of ag50 in *Ascaridia galli*, highly restricted lipid metabolism in nematodes and its affinities to hydrophobic ligands with different metabolic

functions suggest that this novel LBP plays an important role in lipid transport of the parasites and might be involved in parasite-host interactions and for receiving of immunological biopreparations. This work has been presented at IX European Multicolloquium of Parasitology held on July 18-23, 2004 in Valencia, Spain. European Federation of Parasitologists conducts these multicolloquia every 4 years. Concurs of the best presented reports by young scientists was announced. Jury of outstanding scientists awarded the first prize in section "Basic investigations" to PhK student Rositsa Jordanova from the Institute of Experimental Pathology and Parasitology. Her report entitled "Novel Nematode Lipid Binding Protein from *Ascaridia galli*: Structural and Functional Studies" provoked keen interest. Part of the investigations has been conducted in Bulgaria and the other part in the Institute of Tropical Medicine and EMBL, Hamburg, Germany and were financed by the Bulgarian Ministry of Education and Sciences, KAAK, KFG and Marie Curie Training Site-EMBL, Hamburg.

Method for Real-time Communication in the Mother Tongue

Koycho Mitev

E-mail: patentservice@abv.bg; phone: +359 82 272436, mobile: 0887879330, BULGARIA

Constant pursuit of counteraction to threats, overcoming difficulties and discovering new possibilities for development are inherent in human nature. The mankind has sought for resolution of its key problems through known approaches, but more often success has been

achieved by inventing new ones. Contemporary complex and global problems, one of which is international terrorism, may also be approached by other decisions to counteracting.

If we look over the possibilities from scientific and philosophical point of view, they con-

tain two components: cause and effect, mandatory integrated with cause and effect chain. The same refers to political decisions - possible approaches for action here are:

1. Struggle with the consequences of facts, inevitably originating in real life and/or
2. Struggle with the cause of origin of a negative phenomena. The chain of cause and effect is the social and political environment and the degree of information on this environment.

The war with international terrorism from strategic point of view should above all be a struggle with the causes for existence of terrorism. The causes lay in the social environment and its exceptionally limited level of information.

The knowledge about the values of the others is missing. There is a Berlin wall between these two worlds and it should be torn down. Communication between the values is absent. The system of communication is facing the wall of the huge language diversity and impossibility for everyone to learn many foreign languages in order to communicate with the others.

In his book "The Road Ahead" Bill Gates says "...the developed communication systems offer to enlarging the resemblance between the different countries and to diminishing the significance of the national boundaries. The facsimile machine, portable video camera and the cable news network CNN are amongst the powers that forced the end of the communist regimes and the cold war, as due to them became possible for the news to pass through the Iron Curtain in both directions. Most of the information in the Internet now is in English and it will bring economical and entertainment benefits to all around the world who speak English. English-speaking people will enjoy advantages until translation software becomes better and a large amount of content is published in different languages, or until the software starts to handle with the high-ranked task to translate the text in real time."

Eight years ago a team of inventors assigned themselves a task to look for a possibility of organizing **software for real time communication in the mother tongue**, with the help of computing devices.

Please let me enjoy the privilege as a leader of this team to offer to your attention the main technical essence of this solution, which may also appear a powerful weapon to fight the terrorism.

Our solution suggests the use of the already implemented technical decisions based on phone, computer and the Internet.

I would make an effort to explain the essence of the solution, patented by **Patent BG 63704 B1 - 04.10.2002** (Remarkably, exactly on this date John Atanassov, the **Bulgarian who invented the first computer** was born).

The patented invention has a working title *Method for Communication in the Mother Tongue*. Awarding of the patent suggests the availability of three features at the same time:

world novelty, a step ahead in the development of a specific problem, e.g. communications, and industrial applicability.

The invention is industrial property of the authors-claimants. We aimed at checking whether there are common things between all the languages and dialects all around the world. Differences between all the 6800 languages worldwide are obvious. Many of these languages are disappearing and we never think about it. If the process proceeds, we have to create a "Red Book of the Disappearing Languages" in the visible future. The impact of this onto our common future would be even heavier than the extinction of animal and vegetable species.

We should never let this happen.

The aim of the inventors was to find out a common tool to communicate in the mother tongue, which will make all the languages and dialects equal. This kind of communication will permit **tolerant dialogue** between religions, racial and ethnical communities. Right after the awarding of the patent on 04.10.2002, the news was disseminated by the Bulgarian media and by France Press Agency to Canada, Africa, India, Australia, Brazil, etc.

International jury of the exhibition of Inventions, research and innovations, East West Euro Intellect'03 awarded the invention the **John Atanassov Grand Prix**.

The invention is built on the common fea-

tures of human speech, but not on the immense diversities between them. We believe this is the right approach in the political dialogue - to look for what integrates us, not for the differences.

Here are some of the **main features** of the invention:

- The discovered method consists of NEW KIGITAL LITERACY, UNKNkWN BY NkW, common for all the languages and dialects around the world. Mathematics as well as the figures from 0 to 9 carry the same information in all the languages.

- Kigital script is an equivalent computer media to the already familiar graphic means to depict human speech, like Latin, Cyrillic, Greek, Arab, Hebrew, Chinese, Japanese, Korean alphabet, etc. Any other graphic script is equal to the digital computer script.

- Regardless of the language origin, the sentence is the basic component of human speech, which is significant for communication.

- Each kind of human speech contains 10 grammatical partitions: noun, adjective, verb, etc. - exactly 10. Such is the number of the figures: from 0 to 9. Therefore we may cipher the words from each language in figures, so that the nouns are assigned number "1"; "2" for adjectives; "3" for verbs, etc.

- The changeable parts of the words - person, number, gender, tense, etc., will be assigned an appropriate digital code.

- Composition of two and more words, which is a holder of synonymous semantic information, but is not a complete sentence, will be a sum of digital codes of separate words.

- For the needs of syntactic analysis, the computer device will read the initial figures of the words from the completed sentences and after implementing the respective rules for sequence and control from each language grammar, will translate the text in real time, sentence by sentence, in the respective word order.

- The mother tongue communication will be achieved through juxtaposing of the digital codes from one language with those from the other. The software will read only figures in a way the bar code readers identify the numerical bar codes from the package labels of millions of

goods.

- The task for voice recognition has already been given a scientific solution. Now everyone can pronounce to his/her cellular phone the name of the respondent and the device will automatically write out the phone number. In our case, the phone will transcribe into its memory the phonetic equivalent of the words to their digital code.

- Each language and dialect may receive its unique digital code. The device will recognize the words from the relevant language having set the kind of the language, as in case with the country phone codes. The familiar word processing software has also settled this task.

- The device for processing the human speech translation with the help of the digital script may be a small electronic chip, post stamp size, inside the telephone receiver or the microphones, e.g. in the European Parliament or the UN General Assembly. The mother tongue communication via Internet will be achieved in the same way.

- This kind of script is common for the phonetic speech and the speech in writing and this will allow communication in the mother tongue in the modes: voice - to voice; text - to text; voice - to text and vice versa.

The digital script, being an integral part of the method for communication in the mother tongue, according to the patent, is an industrial property. It is **not reasonable** for it to remain a private property. The music notes are common graphic alphabet, and they are not private ownership.

The invention may turn into a tool of communication in the mother tongue having all the languages and dialects fully equal. **The first stage** of accomplishment of the aim is to create a demo model for communication between three or four languages with a digital coding of the words of each language according to the described technology. Let us not leave this only to the software giants, which might do much to embrace our idea, but might do everything to discomfit it. They have



sufficient area to operate.

We would appreciate attracting young people, students and the intellectual elite from different countries to the process of development of software products. They might perform the digital coding **following the matrix** which will be consigned to them. Intellectual elite in each country strongly influences its nation's system of values.

I believe that, provided this elite is given the credibility to achieve something significant for its ethnos, it will do it. The thought for a possible equality of my mother tongue with those of the "the big" or less big nations will create commitment. This newly established environment would struggle against those, who instead of giving support to the concept of equality, look for terrorist tools. This same environment, giving birth to terrorism, may tear down the **21st century Berlin wall**, beyond which the information about systems of values of the others is dimmed. And then such individuals as Martin Luther King might come, saying *I have a dream...*: all the nations, races and religions to be equal.

The notion that every foreigner who doesn't speak my language will have possibility to touch my history and culture, and vice versa, will be an **outstanding motivation** for behavior. Think about the students' motivation, their confidence, when understanding that they might be holders of a part of the Copyright © for the software, allowing their mother tongue to communicate with all the others. And these rights are held 70 years after the death of the last co-author! Both their energy and attention of people from the relevant social environment would be directed to positive expectations and messages.

NATk and politicians from the Balkan region might invest in this invention. Investments in education, in software development, in rewards for the accomplishes are very promising investments. The Balkan countries might **become a model** for such kind of cooperation, focusing at the creation of an environment for communication in the mother tongue. What would be the better field for dialogue of equal rights between the krthodox, Catholic and Islam values?

When speaking about authors' rights, we

have to look in **the maze of the intellectual ownership**. Kuring the recent 14 years, painful processes of shifting the political systems from communism to democracy have been passing. At the same time, the world economy entered global changes. Now intellectual ownership is a political strategy for the economical and social planning of companies, regions, and state governments within the developed countries.

Today, the **colossal difference** between the countries with a high GKP and desperately poor countries is measured by the amount of intellectual property rights from the economic actors. In the developed countries, the market price of small and medium-sized companies is determined by ownership of more than 70% intangible assets in their balance sheets. The share of the fixed assets - immovable and movable, is less than 30%.

The rights over the intellectual property: hi-tech, know-how, trademarks and industrial design, chips topology, patents, new plant's sorts of and animal's breeds are the main engine of economic growth. Intellectual products in the developed countries are also the result of the Brain Krain processes from our region. If you have a look at the statistics of the USA Patent kffice about the number of registered patents from foreign countries, you will notice the discouraging difference between them.

The Balkan countries: Bulgaria, Romania, Serbia and Montenegro, Macedonia, Albania, Croatia, Bosnia are **really drained**. They are at the bottom in the rank of the number of registered patents.

Thousands of young researchers obtain their university degrees here, and now create intellectual products in the USA and Western Europe. The situation in the countries that cradle international terrorism is similar.

The Brain Krain processes cannot be neglected. In this respect, investments in education and in high-tech communication, which undoubtedly our invention is, are **investments in the security** of the Balkan region.

We all desire such a security. Invest in this project. **We believe** this invention will transform our ideas about communications.



EQUAL IN EUROPEAN RESEARCH AREA

BULGARIAN VIPs:

**Academician
DOTCHI EXEROWA, DSc.**

Prof. Exerowa is a highly qualified scientist and researcher with wide international recognition, leader of younger scientists, university professor, and supervisor of many PhK or MSc theses.

Contributions of Prof. Exerowa are mainly in the field of thin liquid films. Many of the results obtained are pioneer results. They have stimulated new directions in the development of knowledge in the field of thin liquid films as well as physics and chemistry of the surface phenomena. In thin liquid films surface forces are acting highly depending on the two phases in contact and determining the formation and stability of the films. Already in the sixties of the past century Professor Scheludko (her teacher) and Kr. Exerowa developed unique experimental methods for liquid films study. The equipment for microscopic thin liquid films investigations is known as microinterferometric technique of Scheludko-Exerowa. The first quantitative assessment of the theory of colloid stability - the KLVk theory, was made. As it is well known, it is one of the first successful quantitative theories of colloid systems stability, which determines to a great extent their development and investigation. Further development of Prof. Exerowa's investigations led to the study of interactions between two phases through the thin liquid film resulting in bilayer contact between them. This serious fundamental problem was solved by the creation of new unique experimental methods, new quantitative experiments and new theories. It is worth to note, that successful development of the experiment is based on the introduction of the model - microscopic horizontal thin liquid film (film radius about 100 μ m). This model allows working at very low surfactant concentration and to study the formation and stabil-

ity of this thinnest liquid formation at the same time.

As it can be further seen, some of the results presented in the considered papers can be directly used in practice. Particularly remarkable is their application in biomedicine.

The main achievements in the presented 174 papers, including 13 review papers and two monographs, can be arranged in groups under several topics.

1. *Unique experimental methods* for thin liquid films study have been developed. They allow to measure important parameters characterizing their properties: equilibrium thickness, critical thickness of rupture, disjoining pressure, contact angle film/bulk liquid, etc. The method for direct measurement of the interaction forces (disjoining pressure) in microscopic liquid films and the transition from long-range to short-range molecular interactions deserves special attention. These methods allow measuring KLVk and non-KLVk forces (i.e. structural, steric). Recently they are used in a number of laboratories all over the world: University of California in Berkley (USA), Technical University of Virginia (USA), Max-Planck Institute of Colloid and Interface Research in Potsdam and Technical University in Berlin (Germany), Moscow State University (Russia), Institute of Surface Chemistry (Sweden), Ecole Normale (Paris), Institute of Food Research (Norwich), etc. Methods allowing investigation of formation and stability of the thinnest black films, including Newton black films, i.e. bilayers, have been created as well. Their investigation was started by Perrin a century ago. Nowadays these methods using modern technique allow investigation of the metastable states at the transition of common

black/Newton black film; forced rupture by α -particles irradiation; FTIR spectroscopy of black films; foam films formation by feeding the surfactant from the gas phase, etc. The parameters determined by these methods give possibility of a new approach to the study of the phenomena at interfaces and small volumes.

2. Surface Forces. A new vision of the electrostatic interactions in liquid films has been developed. For the first time the values of the diffuse electric layer potential at the interface liquid/air and the isoelectric points at this interface have been determined. The critical isoelectric points at the barrier overcoming in the isotherms disjoining pressure/thickness have been determined. These parameters are very informative for the understanding of the charge nature and the electrostatic interaction respectively.

For the first time foam films from liposome suspensions of phospholipids are obtained. Barrier and non-barrier transitions in the isotherm of disjoining pressure are experimentally obtained.

Multilayer foam films from solutions of mixed surfactants in the presence of organic phase are experimentally obtained and a "step like" isotherm of the disjoining pressure is measured. This allows their quantitative study and puts the basis for the study of a new type stabilization of disperse systems.

KLV κ and non-KLV κ surface forces in liquid films from amphiphilic block copolymers (PE κ -PP κ -PE κ type) are determined, i.e. the interaction between two aqueous solution/air interfaces. The results obtained in this direction present certain interest in the field of polymeric investigations. The transition from electrostatic to steric stabilization is found by determination of the critical electrolytic concentration, which divides the two types of interactions. It is found that the electrostatic repulsion arises from the charge at the water/air interface due to the preferential adsorption of κH^+ ions. For the non-KLV κ surface forces - brush-to-brush contact is established and the disjoining pressure isotherm follows the de Gennes scaling theory.

3. Amphiphile bilayers. A new approach to the thinnest black film is developed. A microscopic theory of formation and stability of amphiphile bilayers is created. The rupture of bilayers is considered on the basis of a fluctuation mechanism of formation of nanoscopical holes in the bilayers. The

hole formation is treated as a nucleation process of a new phase in a two-dimensional system with short-range intermolecular forces. Free rupture and deliberate rupture (by α -particles) of bilayers are described. The role of bulk surfactant concentration for formation and stability of amphiphile bilayers is shown. The combination between theories has led to the determination of a number of important parameters, such as the binding energy of amphiphile molecules in the bilayers, and specific hole linear energy, which are important characteristics of the short-range surface forces in bilayers. Also for the first time the equilibrium surfactant concentration has been found, at which the bilayer (in contact with the bulk phase) is thermodynamically stable. In that way the ruptured films, the metastable and stable amphiphile bilayers can be clearly differentiated in good agreement with the theory and experiment.

Occurrence of two-dimensional chain-melting phase transition in foam bilayers was established for the first time. This became possible by the hole mediated theory in accordance with the experimental study of the influence of temperature on the foam bilayer thickness and the critical concentration for formation of foam bilayer. The binding energy of two neighbouring phospholipid molecules was determined for the gel and liquid crystalline state of the bilayers from several phospholipids. Concentration/temperature phase diagrams of KPPC bilayers which contain regions of gaseous (ruptured), gel and liquid crystalline foam bilayers were drawn. It is to be expected that foam bilayers from phospholipids could be used as a model for investigation of short-range forces in biological structures, of interaction between membranes, etc.

4. Bilayer contact in liquid disperse systems. The last stage of interaction between bubbles, particles, droplets, vesicles, etc. in a liquid has been studied by models on basis of the results (theoretical and experimental) of amphiphile bilayers. Differentiation and comparison between the two types of bilayer contact is interesting: amphiphile bilayers from surfactants and brush-to-brush contacts of amphiphilic block copolymers, the latter in agreement with de Gennes scaling theory.

5. New theoretical visions of polyedric foams are developed. They are experimentally verified for solutions of different surfactants, amphiphilic poly-

mers, natural and technological mixtures. Methods for the differentiation of the processes connected to syneresis and stability of foams have been developed. These are the methods for "drainage" and rupture of foams by creating a pressure gradient in the liquid phase. In that way the processes and factors acting in liquid channels and foam films are distinguished. This allows the quantitative study of foam films role and the introduction of new characteristics of their stability. **Applications** - new method and equipment for foam stability determination at constant capillary pressure; methods for rapid rupture; effective foam concentration and separation; water purification from surfactants; foam elimination at waste materials of nuclear fuel processing; effective foam formation at surfactants with high self-stabilizing ability during oil recovery, etc.

6. Self-assembly in thin liquid films. It is interesting to note the investigations that have started in the recent few years related to the amphiphile self-assembly in foam films, i.e. self-assembly process study in the field of disjoining pressure in thin liquid films and its experimental observation as a block pattern formation in the low concentration range of the surfactant solutions.

7. Wetting films. Another very useful direction of Prof. Exerowa's investigations is the parallel studies of foam and wetting films from aqueous cationic surfactants and amphiphilic block copolymers. Parallel investigation of symmetric and non-symmetric thin liquid films shows that the electrostatic interactions between identical or different interfaces could differ when the surfactant concentration is varied, and the transition from electrostatic to steric interactions is established for the cases of wetting films.

8. Lung Surfactant System. A study of the lung surfactant system is carried out on the basis of theoretical and experimental investigations of amphiphile bilayers from amniotic fluid and alveolar surfactant. A new in vitro model to study alveolar surface and stability, namely a microscopic foam film method, is introduced at the conditions in the lung alveolus: capillary pressure, radius, electrolyte concentration and temperature. It is shown that at

these conditions a foam bilayer stabilized by short-range interaction forces is formed and new parameters characterizing its formation and stability are introduced. On this basis new clinical methods for diagnosis of lung maturity and assessment of surfactant lung maturity of newborns are created. The very good fit of the clinical results and the parameters of the in vitro model have allowed creating a new hypothesis for the structure of the alveoli, namely ordered structure in the contrary to the widely accepted "monolayer" model. The most significant feature of the offered new model for the alveolar structure is that its stability is determined by the lateral short-range interactions as well as by the normal interactions between the ordered molecules. This gives possibility for quantitative study of the lung surfactant system, and the processes related to the main physiological process - breathing. **Applications.** The new created method for fetal lung maturity assessment has a number of advantages: high precision (90%), small quantity of liquid used (1 cm^3), very fast - the result is ready in about 20 minutes. It is used for research purposes in Medical University of New Jersey (USA), University Clinic "La Sapienza" (Rome, Italy), University Clinic (Sofia), etc. The method for lung maturity diagnosis is also very successfully developed for therapy control, i.e. defining the action of therapeutic surfactants, which cure the respiratory distress syndrome. The correlation between the experimentally determined parameters and their in vivo action is found. This creates possibility to look for the most effective medicines to influence the lung surfactant system at respiratory distress. Famous American physiologist Prof. Scarpelli supports this in his article "Rapid in Vitro Tests of Surfactant Film Formation: Advantages of the Exerowa Black Film Method", *Pediatric Pulmonology*, 21 (1996) 373 (a copy is enclosed).

It is worth noting that the scientific results of Prof. Kotchi Exerowa and co-workers are well accepted in the international specialized literature (there are over 2000 citations) and at international conferences. A number of plenary or invited lectures have been delivered.

Professor
GEORGY FOTEV, DSc.
sociologist

Professor Georgy Fotev is an eminent Bulgarian sociologist, the author of more than 200 scientific publications, among which more than 20 books. Publications by him have come out in 15 countries besides Bulgaria.

His main scholarly contributions are in the fields of history and theory of sociology and a number of disciplines of contemporary sociology. He has presented original arguments in support of the poly-paradigmatic character of modern sociology and has particularly focussed his research on a very difficult problem, that of the incommensurability between sociological paradigms, as a result of which he has come to view sociology in a dialogical perspective. With regard to the cleavage between the sociological paradigm treating of social reality as of "things" and that which views it as a subjective construction of the social world in terms of meaning, the author opposes the view that the two paradigms are mutually complementary. He has made important contributions to historical sociology, to the problem of the periodic legitimacy crises in modern societies, to the field of ethnosociology, sociology of religions, etc. In the large-scale treatise entitled "Limits of Politics", he has studied fundamental problems of the civil society of modern democracy, of social conflicts, social inequalities, etc. His latest monumental work "Dialogical Sociology" has met exceptional interest in the academic community of specialists.

Prof. Fotev's more important books are:

Sociological Theories of E. Durkheim, W. Pareto, M. Weber (1979);
Principles of Positivist Sociology (1982);
Social Reality and Imagination (1986), 2nd. edition 1996, translated into Greek 1996;
Civil Society (1992), translated into Greek 1996;
History of Sociology in two volumes (1993); 2nd edition 2000;
The Other Ethnos (1994);
Crisis of Legitimacy (1999);
The Meaning of Politics (1999);
Ethnicity, Religion and Politics (1999);
Limits of Politics (2001);
Dialogical Sociology (2004).

In the time of the totalitarian communist regime, Prof. Fotev met with difficulties in his academic career. After the democratic changes in Bulgaria, he was for many years the Director of the Institute of Sociology of the Bulgarian Academy of Sciences. He has also had a long teaching career in the University of Sofia St. Kliment khridski (reading courses in the history of sociology, sociology of religion, epistemology of sociological knowledge, dialogical sociology). He was Minister of Science and Higher Education (1991) and is a member of the European Academy of Sciences and Arts, as well as of a number of other prestigious international organizations. He has been a guest lecturer at foreign universities.

AWARDS

**The Minister of Education and Science
awarded the following prizes for encouraging scientific research for 2004:**

1/ In the field of the social and humanitarian sciences - to Academician **Vassil Todorov Gyuzelev**: an honorary diploma for special contributions to science, a plaque of the Ministry of Education and Science and a financial prize.

2/ In the field of the medical sciences - to Associate Professor Kr. **Yordan Dimitrov Dimitrakov**, Kr. of Med. Sc.: an honorary diploma for special contributions to science for 2004 for young scientist up to 35 years of age, a plaque of the Ministry of Education and Science.

**The Evrika Foundation
awarded the following prizes for 2004:**

For achievements in science

IVANKA MILOSHEVA TSAKOVSKA

Central Laboratory for Biomedical Engineering, Bulgarian Academy of Sciences, BAS

Ivanka Tsakovska was born in 1972 in Radomir. She has graduated from the Chemical-Technological and Metallurgical University in Sofia with the qualification of engineer-chemist. She has worked as a technologist at "Medbioengineering" Ltd. Since 1997 she has been a full-time Ph.D. student at the Central Laboratory for Biomedical Engineering of BAS. Since 2002 she is a research associate (II rank), continuing to work in the same laboratory.

Ivanka Tsakovska participated in research teams for scientific projects, financed by the National Fund "Scientific Research". She was awarded the first prize in the competition "Young Scientists 2002". She has given lectures on eleven scientific forums, nine of which were with international participation. In 2001/2002 she was awarded a scholarship by the Alexander von Humboldt Foundation. She has eleven scientific publications and is a member of the professional scientific organization The

QSAR and Modeling Society. Mrs. Tsakovska receives the joint award of the Evrika Foundation and the Higher Attestation Committee at the Council of Ministers for the excellent defence of the dissertation "Quantitative structure activity relationships (QSAR) of selected classes of biologically active compounds", for which she is awarded the educational and scientific degree Kotor. Through classical QSAR approaches and molecular modelling approaches, in her thesis she has examined selected classes of biologically active compounds of principal importance for pharmacological and clinical practice. QSAR models have been built for quantitative characterization of the influence of structural parameters on the biological activity of the compounds, receiving of more information on the molecular mechanisms of activity of the investigated compounds and for directing the rational construction of new active compounds.

For young inventor

DIMITAR IVANOV NIKOLOV

Institute of Control and System Research, BAS

Kimitar Nikolov was born in 1975 in Sofia. He has graduated from the Technical University in Sofia with specialty "Microelectronics". Since 2000 he has been working at the Institute of Control and System Research of BAS, consecutively as an engineer-researcher, research associate III rank, re-

search associate II rank and research associate I rank. His professional interests are in the sphere of sensors and microsystems for magnetic field and temperature.

Mr. Nikolov was awarded the ICSR prize for best scientific publication for 2000, and in 2002 he

received the prestigious BAS award for the youngest scientist up to 30 years of age in the field of technical sciences. The prize "Evrika" is awarded to Kimitar Nikolov for his invention "High-temperature Hall Sensor with Parallel Axis of Sensitivity". The purpose of the invention is to eliminate the existing parasitic pressure of unequipotentiality through balancing of the potentials inside of the pad and to achieve their equality on the two outgoing plugs. The advantages of the invention are the increased accuracy of measuring of the magnetic field and the possibility of high-temperature (up to 400 C) functioning of the Hall sensor. It can be applied in the control measurement technology, tool-building industry, high-temperature electronics and electrical engineering, automobile electronics, no-contact au-

tomatics and military science. The scientific-applied effect of the invention is connected with increasing the knowledge about technologies of magnetosensitive sensors and microsystems, and the expected economic effect of its introduction is around 500 000 lv.

With his colleagues from the Institute of Control and System Research Kimitar Nikolov is a co-author of 7 more inventions that are awaiting patents.

In the young inventor competition honorary diplomas for excellent performance are awarded to Bistra Markova from Vratsa, Krassimir Ganey from Rakitovo, Bogdan Rangelov, Emil Stoyanov and Viktoria Gentcheva from Sofia.

For young manager

HRISTO TEODOROV ILIEV

Chairman of the Board of Directors of "Address Bulgaria Holding" Ltd.

Hristo Iliev was born in 1972. He holds a Bachelor's degree in "Economics and industrial management" and a Master's degree in "Marketing" from the University of Economy in Varna. He started his career in 1993 in the field of real estate as a consultant, passed through management of one of the AKKRESS offices and since 1996 has been the Chairman of the Board of Directors of "AKKRESS Bulgaria Holding" Ltd.

Mr. Iliev is one of the founders of the first Bulgarian real estate index REM1. He is the winner of the award for considerable contributions to the development of the profession, awarded to him by the National Real Estate Association. Hristo Iliev is one of the three Bulgarians, owning the international license CIPS, giving him the right to make deals on an international scale.

The company headed by Mr. Iliev distinguishes itself from the others in the real estate branch with its national scope, its modern information system connecting the offices in real time, implemented systems for education and development of the staff, achievements in the field of marketing and advertising, information technologies, and raising the quality of the offered services. Thanks to the application of its business models AKKRESS is already represented in 8 cities

(a growth of 125 % compared to 2003), owns 55 offices (a growth of 111% compared with 2003) with staff of over 500 people (a growth of 97%), and has increased its turnover by 120 %. In 2004 the company structured an international section responsible for penetration not only into traditional markets such as Great Britain and Ireland, but also Russia, EU, the Far East and the USA. The company presented itself exceptionally successfully at the first Bulgarian real estate fairs "Imoti Expo" and "Kve strehi", as well as at fairs in Great Britain, Hungary and France. In September 2004 AKKRESS opened an office in London, and in November successfully completed the ISO 9001:2000 certification process.

The company is a long-standing member of the following prestigious organizations: National Real Estate Association (NREA), Bulgarian International Business Association (BIBA), American Chamber of Commerce in Bulgaria, Italian Chamber of Commerce in Bulgaria, CEREAN, FIABCI, REALT.R.

For their excellent performance in the national competition, Slavin Dimitrov Yanakiev (chief executive of "Progress" Ltd. - Stara Zagora) and Dimitar Milanov Badzhov (chief executive of ICYGEN) are awarded honorary diplomas.

RECENT PUBLICATIONS OF BULGARIAN SCIENTISTS

ARTICLES

Title: **Computational Challenges in the Numerical Treatment of Large Air Pollution Models**
Authors: Kimov, I. 1), Georgiev, K. 1) Georgiev@parallel.bas.bg, kstromsky, Tz. 1), Zlatev, Z. 2)
Source: Ecological Modeling, Vol. 179, 2 (Nov. 2004), 187-204
Author Affiliations: 1) Institute of Parallel Processing, Bulgarian Academy of Sciences, Acad. G. Bonchev Street, Bl.25-A, 1113 Sofia, Bulgaria
2) National Environmental Research Institute, Frederiksborgvej 399, P.k. Box 358, KK-4000 Roskilde, Denmark

Title: **Modelling the Influence of Conductivity Profiles on Red Sprite Formation and Structure**
Authors: Tonev, P. T. ptonev@bas.bg, Velinov, P. I.Y.1)
Source: Advances in Space Research, Vol. 34, 8 (oct. 2004), 1792-1798
Author Affiliations: 1) Central Solar-Terrestrial Influences Laboratory, Bulgarian Academy of Sciences, Acad. G. Bonchev Street, Bl. 3, 1113 Sofia, Bulgaria

Title: **Moessbauer Transmission and Back Scattered Conversion Electron Study of Fe Nanowires Encapsulated in Multiwalled Carbon Nanotubes**
Authors: Ruskov, T. 1), Assenov, S. 1) Spirov, I. 1) Caria, C. 1) Moench I. 2) imoench@ifw-dresden.de, Graff A. 2) Kozuharova, R. 2) Leonhardt, A. 2) Schneider, C. M. 2), Groudeva-Zotova, S. 2)
Source: Journal of Applied Physics; Vol.96, 2 (Kec. 2004), 7514-7519,
Author Affiliations: 1) Institute for Nuclear Research and Nuclear Energy, 72, Tsarigradsko Chaussee, BG-1784, Sofia, Bulgaria 2) Leibniz Institute of Solid State and Materials Research, Kresden, Helmholtzstrasse, Germany

Title: **New Index to Remove from Spectral Mixture an Unknown Spectral Component**
Authors: Yanev, T. K. 1) Choudhury, B. J. 2) Mishev, K. N. 1)
Source: Acta Astronautica, Vol. 56,4 (Feb. 2005), 471-476,
Author Affiliations: 1) Solar-Terrestrial Influences Laboratory, Bulgarian Academy of Sciences, Acad. G. Bonchev Street, Bl.3, 1113 Sofia, Bulgaria 2) NASA Goddard Space Flight Center, Code 974, Greenbelt, MK 20771, USA

Title: 3D QSAR Investigation of the Blood-brain Barrier Penetration of Chemical Compounds

Authors: Lessigiarska, I. 1, 2) iglika.lessigiarska@jrc.it
Pajeva I. 3), Cronin M. T. K. 2) Worth, A. P. 1)

Source: SAR & QSAR in Environmental Research, Vol. 16, 1/2(Feb. 2005), 79, 5 charts, 2 diagrams

Author Affiliations: 1) ECVAM, Institute for Health and Consumer Protection, European Commission Joint Research Centre, 21020 Ispa, Italy 2) School of Pharmacy and Chemistry, Liverpool John Moores University, Byrom Street, Liverpool L3 3AF, UK, 3) Centre of Biomedical Engineering, Bulgarian Academy of Science, 1113 Sofia, Bulgaria

Title: Investigation of the Retaining Effect of a Pectin-Containing Edible Film upon the Crumb Ageing of Dietetic Sucrose- Free Sponge Cake

Authors: Baeva, Marianna 1)mbaeva@doctor.bg Panchev, Ivan 2) ivanpanchev@hotmail.com

Source: Food Chemistry, Vol. 92, 2 (Sept. 2005), 343-349.

Author Affiliations: 1) Technical University of Sofia, College in Sliven, 59 A Bourgasko Chaussee Blvd., 9800 Sliven, Bulgaria, 2) University of Food Technologies in Plovdiv, 4002 Plovdiv, Bulgaria

Title: Moisture Sorption Characteristics of Chickpea Flour

Authors: Kurakova, Albena G. 1) aldurakova@yahoo.com Menkov, Nikolaj K. nimenkov@hiffi-plovdiv.acad.bg

Source: Journal of Food Engineering, Vol. 68, 4 (Jun2005), 535-540

Author Affiliations: 1) Department of Process Engineering, University of Food Technologies, 26 Maritza Blvd., 4200 Plovdiv, Bulgaria

Title: Visual Modeling as a Motivation for Studing Mathematics and Art

Authors: Sendova, Evgenia 1) jenny@math.bas.bg, Grkovska, Slavica 2)

Source: Educational Media International, Vol. 42, 2 (Jun. 2005) 173-191

Author Affiliations: 1) Bulgarian Academy of Sciences, Bulgaria, 2) Institute of Mathematics, Republic of Macedonia

Title: Rotation of the Cluster of Galaxies A 2107

Authors: Kalinkov, M. 1) markal@astro.bas.bg, Valchanov, T. 1) tony@astro.bas.bg, Valtchanov, I. 2) i.valtchanov@imperial.ac.uk, Kuneva, I. 1) Kissanska, M. 1)

Source: Monthly Notices of the Royal Astronomical Society; Vol. 359, 4, (Jan.2005), 1491-1498.

Author Affiliations: 1) Institute of Astronomy, 72 Tsarigradsko Chaussee Blvd., Sofia 1784, Bulgaria, 2) Blackett Laboratory, Imperial College, Prince Consort Road, London SW7 2 BW



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E-Mail: infobg@hotpop.com,

ICQ#: 295588455

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Bulgarian Academy of Science

Address:

Secretariat Bureau

14,"Kliment khridsky" Blvd.

1797 Sofia, BULGARIA

Phone: +359 2 975 3982 (+ voice mail box)

Fax: +359 2 817 2477

E-mail: sgem@sgem.org, sgem@stef92.com

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GSM: +359 8 99944410

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ICQ#: 295588455

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E-mail: furnadjieff@math.bas.bg
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1 J. Boucher Blvd., 1126 Sofia, Bulgaria
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GSM: +359 8 999 444 10
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8, Kl. khridski blvd., Sofia 1000, BULGARIA,
Assoc. Prof. Plamen Tzvetkov, PhK
E-mail: tzvetkov@tu-sofia.bg
Phone: +359 2 965-2366;
Assoc. Prof. Ivan Kodjabashev, PhK
E-mail: kodjabashev@tu-sofia.bg
Phone: + 359 2 965-2438
Fax: +3592 683215
E-mail: metrology@tu-sofia.bg
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Address:
kffice H-108; University of Economics
N 77, „Knjaz Boris I“ Blvd.
9002 Varna, Bulgaria
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+ 359 52 602 417
e-mail: tourism@ue-varna.bg
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