SECTION 1: PRESIDENTS' ADDRESSES

MEBC: From Past To Future

Michael Conrad
Immediate Past President
ISMEBC

For the past three years I have had the pleasure, and the honor, of helping to form the ISMEBC. Actually the work of organization runs back to the initial meeting organized by Géza Biczó in Hungary in 1987 [1]. We wrote up a draft of the constitution at the Moscow meeting (organized by Pavel Lazarev) in 1989 [2].

The Society was officially inaugurated at a subsequent meeting in Balatonszéplak, Hungary in 1991, organized by Géza and by Péter Rajczy. Géza was elected first President and a Board of Governors was elected. I was chosen as President-Elect and Robert Birge was elected as a Vice President (to fill the position that would eventually be occupied by Immediate Past President).

The meeting at Balatonszéplak was designed to put the Constitution of the Society together and to get the infrastructure formally set up, but of course we also wanted a scientific meeting. The science eventually appeared in a special issue of BioSystems [3]. None of us can claim to be experts on putting organizational structures together. In retrospect it is easy to see there are some holes in our structure and some unclarities on how to best interpret the procedures. No matter. The spirit is there, and the little holes will get fixed up.

The real question is, what kind of structure will best serve? Our framework leaves this open to a considerable extent. We could end up with a centralized organization, with a lot of chapters supporting and supported by that center. Or we could end up with a highly federated group of chapters, each a tub sitting on its own bottom, with a central administration that moves from one chapter to another and that mainly has the job of keeping the meetings and communication links alive.

So far we have emphasized the decentralized model, with local representatives (points of contact) handling local dissemination of information and organizing local activities. The reason is simple: the situations in different regions are just so diverse and the world is changing so rapidly that flexibility and adaptability are all important. In a field such as ours, where there is a great deal of promise and spirit, this will probably work best.

There are a couple of centralized functions that it will certainly be necessary to cultivate further. So far the main activity has been the meetings. The first meeting held after the formation of the Society (but decided on already at the Moscow meeting) was organized by Robert Birge in the framework of an American Chemical Society meeting in New York in 1991 [4]. The first meeting actually planned by the Society subsequent to its formation was held in Gaithersburg (near Washington DC) in 1993 and co-sponsored by the National Institute of Standards and Technology. I want to take this opportunity to express my gratitude to all those who made this meeting a success and who contributed to the Proceedings, which appeared as another special issue of BioSystems [5]. The third meeting, organized by Girjesh Govil and Ratna Phadke, was held in Goa, India, 1994.

The fourth meeting, to be held jointly with the biennial Future Electron Devices (FED) meeting on bioelectronic and molecular electronic devices and being organized under the Presidency of Masuo Aizawa, will be held in Okinawa in November, 1995. It promises to be a signal event.

The movement of meeting sites back and forth between Europe, the U.S., and the Far East has served to facilitate communication and bring new investigators into the field, expose students to the possibilities, and provide a forum for new developments. The publications have helped to create a field per se—after all, not more than a decade ago scientific papers in the field were lost in disparate journals and most of the accessible reports were actually in the popular press. Now a substantive literature exists, and some definite fora have emerged that target suitable audiences.

Still, it is probably fair to say that the Society needs its own journal, and I would suggest that this should be one of the immediate goals. The Newsletter is already in place, and might evolve into such a journal. The electronic network being organized by Péter Rajczy and Klaus-Peter Zauner, will undoubtedly play a major role. In short, it seems to me that we should pursue the decentralized (chapter, points of contact) model, but at the same time develop an ongoing center that can keep the ball rolling.

As to science, I can only say that I regard the progress as dramatic. I recall two early meetings, one on chemically based computer design held in Santa Monica in 1983 (organized by Eugene Yates, of the Crump Institute at UCLA, with myself as co-organizer) and the first Future Electron Devices meeting on bioelectronic and molecular electronic devices held in Japan in 1985. At both meetings the question came up, when will there be molecular devices that subserve significant computational or information technology functions? In Santa Monica I thought maybe 50 years, pretty fast on an evolutionary time scale from my point of view. Evidently this seemed rather distant to the group of roughly fifty newspeople that UCLA public relations had set loose on me. At the FED meeting I could see that the effort would be more concerted. I lowered my estimate to ten years. And indeed in the past decade real prototypes have come to be. Bacteriorhodopsin has been tamed for tasks. Biosensor technology has increased enormously. A variety of optomolecular prototypes are extant. DNA computing has been initiated. General principles have been delineated, and new virtual (neuromolecular) designs have been explored which are good candidates for usefully assimilating molecular electronic technologies.

But I think the most dramatic fact is my distinct recollection of what has happened to the impossibility arguments. They have been consigned to the trash can. I could go through a long list of reasons given by the naysayers as to why organic and bio-organic molecules could not cut the ice for computing. But always some investigator, from biology, or chemistry, or engineering, or physics or from one of the hybrid fields, came along with some idea that just bypassed that objection. Usually the bypass was not direct. It was just an idea that did not even occur in the objector's universe. And I expect this general trend to continue.

It is important also to acknowledge the contributions that efforts in our field have made to a deeper understanding of general principles of information processing, both as they apply to biological systems and to computer science, and to the biological foundations of computing. The theoretical understanding of both fields has been deepened and expanded. The measurement techniques that have been developed in the context of molecular electronic technologies are providing new and powerful ways of looking at nature. New classes of materials, devices, and architectures are being developed, along with new paradigms and new concrete models for understanding the brain and other natural biological processes. It is a mutually self-facilitating process. Thirty years ago even the nascency of the field was barely detectable. In 1995 we can see that for the past decade and a half we have been on the early upswing phase of a growth curve, one whose dramatic significance probably will only be fully perceivable by future historians.

MEBC Meeting Publications

[1] J. Molecular Electronics, Vol. 4, No. 1, 1988. This is a special issue devoted to the first symposium on Molecular Electronics and Biocomputers, ed. by G. Biczo and P. Rajczy. Additional articles from the symposium are in subsequent issues.

[2] Molecular Electronics: Materials and Methods, P.I. Lazarev, ed., Kluwer Academic Publishers, The Netherlands, 1991.

[3] Proceedings of the Workshop and Initial Meeting of the International Society for Molecular Electronics and Biocomputing, BioSystems, Vol. 27, No. 4, G. Biczo and P. Rajczy, ed., 1991.

[4] Molecular and Biomolecular Electronics, R.R. Birge, ed., Advances in Chemistry Series 240, American Chemical Society, Washington, DC, 1994.

[5] Proceedings of the 1993 Meeting of the International Society for Molecular Electronics and Biocomputing, BioSystems, Vol. 35, Nos. 2,3, M. Conrad, ed. chair, 1995.

See also **EDITORIAL,** *Inside Back Cover*

PRESIDENT'S ADDRESS

Mike Petty
President ISMEBC

Dear Colleagues,

It is a privilege to be elected as your President for 1996. Molecular electronics and biocomputing are now 'hot' research topics and it is important that our Society continues to be active in their promotion. I have a very short time in office but have identified some areas in which I hope we can move forward in the next twelve months.

Perhaps the most important matter concerns publications. Here, ISMEBC has several specific goals. These include getting a major publisher interested in this Newsletter; introducing 'MEBC Letters'; and finding a regular outler for our conference proceedings. Much work has already been done by previous Presidents. I am actively following this up and now am involved in discussions with a leading publisher.

Another very major Society activity is our conference. Currently, there is a proliferation of meetings covering molecular electronics and biocomputing. I hope to establish links with some of the organisations responsible for these so that we can plan joint conferences in the future. However, the next international conference of ISMEBC will be in Nanjing, China, 10-12th November 1997. Put the dates in your diary now.

Our current membership stands at several hundred. We can increase this significantly. I would especially like to recruit more industrial members. You can all help by drawing colleagues' attention to our activities. A very useful way of doing this is to advertise widely our Home Page on the World Wide Web (http://mebc.elte.hu/mebc/). I also intend to produce a short advertising brochure that can be made available at appropriate meetings.

There is some news on new officers of ISMEBC. I would like to welcome Dr. Tim Richardson of Sheffield University as our new Treasurer. Tim takes over from Ann Tate who has done a splendid job over the last few years. No doubt, Tim will be after our subscription soon! The Nominating Committee has also been reorganised under Ratna Phadke as the new Chair. The Vice-Chair is Dr. Bruce Gaber (Naval Research Laboratory, Washington) and other committee members are Professors Rambidi, Biczó, Nešpůrek and Rishpon. This committee will shortly be organising elections for Governing Body Members and the next President. Finally, I would like to thank members of the GB who retired at the end of 1995: Bozio, Kahn, Metzger and Rajczy.

SECTION 2: REGIONAL REPORTS

RECENT ACTIVITIES ON BIOMOLECULAR ELECTRONICS IN KOREA

In 1996 we would like to make a turning point of biomolecular electronics researches in Korea. Although some researchers have worked on biomolecular electronics for several years and the 6th Molecular Electronics and Devices Symposium was held at Taejon, Korea in 1995, the Korean researches had been by no means well-funded. Their activities had not been coordinated, and could convince neither government nor industries of the big future of biomolecular electronics. However, it is now changing. A new initiative had started at Korea Advanced Institute of Science and Technology (KAIST) in 1995. To promote researches on biomolecular electronics an interdisciplinary research team was formed from several departments including Departments of Biology, Chemistry, Chemical Engineering, and Electrical Engineering. About 10 professors agreed to join the team. Although several new research projects may start in the near future, the team is currently working on 3-dimensional optical storage systems based on new biomolecular materials. It started on January 1996, and is expected to go for the next 5 years. The project is still at its early initial stage, and we can only summarize its current research goals here.

Although bacteriorhodopsin(bR) and its radicals have been investigated for both 2-dimensional holographic storages and 3-dimensional digital data storages, still more researches are necessary for practical applications. We may need new materials with better optical properties, stability, and mass producibility. Also optical systems need to be improved to take advantage of the biomolecules while maintaining rigidity and compactness. Therefore, the project consists of 4 research topics, i.e.,

1. search for new biomolecular materials,
2. purification and production,
3. characterization and device fabrication, and
4. optical storage systems.

(1) Search for New Biomolecular Materials

We would like to find new biomolecular materials as well as new radicals based on the bR. Biomolecules with better optical properties are expected. In addition to the photochromic property we may also look for photorefractive and electro-optic properties. Genetic engineering technique is employed.

(2) Purification and Production

Processing technique is being developed for high density and high throughput productions of biomolecular materials including bR and other halophilic bacteria. Effects of processing parameters on production performance are investigated for two-stage continuous reactors. Possibility of mass production will also be investigated in the future.

(3) Characterization and Device Fabrication

State transition and photochromic properties of bR and its radicals are investigated. Effects of additives to the transition and lifetime as well as optical properties are studied. Fabrication of thin films and its characterization will be done later. New spatial light modulators may be developed based on the developed biomolecules and thin film structure in the future.

(4) Optical Storage Systems

Optical read/write systems will be designed and tested. Both distributed holographic content addressable memory and location addressable memory schemes are investigated. For the location addressable memory scheme, the addressing may be done at a pixel, a line, or a plane. Also, optical devices such as multi-focus lens may be developed for the system. The system should take advantage of new optical properties of the developed biomolecules for much higher density, lower interference, and lower power consumptions.

Soo-Young Lee, POC Korea

BIO-MOLECULAR ELECTRONICS IN ISRAEL

Recent developments in Molecular Electronics brought about a growing interest in the possibilities to utilize biological molecules in this area and, particularly, in artificial intelligence systems. The pertinent activity is based on the understanding that one should be able to take advantage of the specific characteristics and unique capabilities of these natural molecules, and this view lead to the establishment of Bio-Molecular Electronics as a special field of activity.

In Israel, the main activity in Bio-Molecular Electronics is carried out by Prof. Noah Lotan and his research group, which includes the graduate students S. Tuchman, G. Ashkenazi, S. Nehamkin, S. Sivan and O. Filo. This group operates at the L. & D. Sherman Biomaterials Research Center, in the Dept. of Biomedical Engineering of the Technion – Israel Institute of Technology in Haifa.

The research activities of this group address four main topics:

a) Bio-Molecular Switching Elements: This part of the research focuses on the design and operation of bio-molecular switching elements and, particularly, on enzyme-based ones (ENMOSEs). The functioning of such elements relies on changes in their three-dimensional conformation, as induced by optical signals and/or soliton phenomena. Studies were first addressed to the design of ENMOSEs in which a molecular switch, when attached to an enzyme at appropriate location near the active site area, allows or prevents the access of substrate. As a result, control of the catalytic activity of the enzyme is achieved, thereby creating a bio-molecular switching element. The design involved molecular mechanics and molecular modeling techniques, and used lysozyme as model enzyme.

b) Enzyme Based Logic Gates (ENLOG's): These elements represent a stage of higher complexity in Bio-Molecular Electronics. The research involves the development of concepts and approaches, as well as related experimental work. In this context, systems were developed which implement logic gates, such as AND, OR, NOT, NAND, and NOR. In particular, the optically-actuated logic gates studied involve either the use of two enzymes, each modified so as to respond to different optical signals, or two derivatives of the same enzyme, each carrying different photoreceptor moieties. Another ENLOG configuration investigated involves a modified enzyme and an optically actuated inhibitor. In all cases, the input information is transferred into the gate upon appropriate illumination of the system, and translated into changes of either the activity (ON or OFF), or the level of activity (threshold) of the enzyme. These changes are subsequently processed into logic output, using the basic definitions of the pertinent logic gates, and threshold value concepts.

c) The Interaction of Enzymes with Electroactive Polymers: This investigation is directed at establishing the background required for building an information transfer system which will operate by addressing electronic flow to and from an enzyme, and will do so by using electroconductive polymers as "molecular wires". In this work, of particular interest are polymers which are water soluble, and do not carry additional ionizable groups. To this aim, an appropriate derivative of polyaniline was synthesized, and its intersections with redox enzymes (glucose oxidase, uricase, xanthine oxidase) were investigated. The results obtained clearly indicate that these interactions are very sensitive to the detailed chemical and physical structure of the polymers.

d) Neural Network-type Bio-Molecular Systems: The study addressed itself to the possibility of building biochemical systems which will perform complex information processing functions. Biochemical systems have the advantage of using the "language" of the physiological processes, i.e. the biochemical reactions. As such, they can be organized into neural network-type assemblies, much in the way that natural biosystems are. The basic system considered is designed to function as a "node" in biochemical neural nets. This system involves two enzyme-catalyzed reactions, coupled to one another by the use of a co-substrate continuously cycled between the two. In addition, there are two consumable substrates which are continuously fed into the system at predetermined time course of concentration profiles. A higher level of organization was subsequently achieved by using several basic systems of the type mentioned above, and connecting them in neural network-type arrays. Analytical models were written for these networks and, using numerical simulation techniques, it was found that the characteristics of the output signal obtained depend on the number of basic systems involved and their particular mode of interconnection. Parallel experimental studies, using Glucose-6-Phosphate Dehydrogenase and Glutathione Reductase, confirmed the theoretical predictions.

Noah Lotan, POC Israel

MEBC SITUATION IN RUSSIA

Activities in the field of molecular electronics and biocomputing in Russia were not high in 1994 because of very restricted funding.

Nevertheless main scientific groups specialized in this field (see previous MEBC Newsletters) has been performing experimental and theoretical works.

Some results of these activities were presented at the International Conference on Optical Memory and Neural Networks which has been held in Moscow (August 1994, Prof. A. Mikaelian Conference Chairman).

Between them were:

Nonlinear properties of a crown-bearing dye: optical addressing system on its basis
— G.Matevosov, A.Mikaelian, V.Salakhutdinov;

Molecular electron-transfer memory
— V.Kitovich;

Implementation of neural networks at the molecular level: principles and designing versions
— N.Rambidi, A.Maximychev;

Future improvements in information capacity of recording media
— V.Barachevsky;

Designing hierarchy neural-like system for composite video image processing
— V. Yachno;

Image processing by oscillator media
— Yu.Balkarey, A.Cohen, W.Johnson, M.Elinson, M.Evtikhov, P.Petrov.

The special issue of the Journal *'Optical Memory and Neural Networks'* (New York, Allerton Press, Inc.) on *'Nonlinear Dynamic Mechanisms of Information Processing and Biocomputing'* has been prepared in 1994. This issue was published in the first half of 1995 (vol.5, No2. M.Conrad and N.Rambidi guest co-editors).

Nicholas Rambidi, POC Russia

SECTION 3: SCIENTIFIC ARTICLES

RADIATION CHEMISTRY OF BIOLOGICAL MOLECULES WITH REFERENCE TO MOLECULAR ELECTRONICS AND BIOCOMPUTING

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ABSTRACT

By irradiating aqueous solutions with ionizing radiation, it is possible to generate a wide variety of radicals, many of which are also present in living systems. By using both steady state and time resolved techniques, it is possible to study the reactions of these radicals with a wide variety of biological molecules. These reactions tells us not only about the physiology and biochemistry of these molecules but also about the complex molecular electronics in biological systems and also how biological molecules react intelligently to the environment.

INTRODUCTION

The intention of this short review article is to initiate collaborations between radiation chemists and molecular electronics specialists.

When ionizing radiation passes through water, the following are the main radical species produced.

- (i) e^-_{aq} (the hydrated electron),
- (ii) $OH^\cdot$ (the hydroxyl radical) and
- (iii) H (the hydrogen atom).

The molecular products are H_2 and H_2O_2. In the presence of oxygen and additional radical species, $O_2^{\cdot-}$ (HO_2), frequently called the superoxide radical, is produced.

Out of the species listed above, $OH^\cdot$, H_2O_2 and $O_2^{\cdot-}$ are known to take part in biological processes. Some other species like the radical ion $CO_2^{\cdot-}$ which are present in living systems can be generated radiologically by adding special solutes.

Therefore, it becomes possible to simulate many biological oxidation and reduction processes in very simple aqueous systems using radiation chemical techniques. Using this technique one can gain a much better understanding of these reactions as compared to the direct study of complex biological systems. A great deal of work has been done in this field during the last two decades.

However, what has not been realized so far is that the study of radical reactivities with biological molecules can not only provide kinetic and product data, but also can provide insight into the complex molecular electronics of biological systems.

In the present paper, a few typical systems, studied by the pulse radiolysis technique are presented. The bulk of this work has been carried out in the chemistry division of the Bhabha Atomic Research Centre.

Some typical systems

The toxicity of halocarbons, especially chloro- fluoro carbons (CFC) is now well known. Time resolved radiation chemistry, using the pulse radiolysis technique gives a unique method for assessing their relative biological activity (and hence their toxicity). It is known that in living systems the halocarbons undergo a one electron reduction, loosing a halide ion and giving a radical which then reacts with O2 to give a haloperoxyl radical. It is the reactions of these radicals with biological compounds that causes their toxicity. Carbon tetrachloride can be considered as a typical example.

$$CCl_4 + e^-_{aq} \rightarrow CCl_3^\cdot + Cl^- \qquad (0.1)$$

$$CCl_3^\cdot + O_2 \rightarrow CCl_3OO^\cdot \qquad (0.2)$$

$$\begin{aligned} &CCl_3OO^\cdot + biological\ compounds \rightarrow \\ &\rightarrow one\ electron\ oxidation\ products \end{aligned} \qquad (0.3)$$

The rate constants for the reaction (3) can be measured using the technique of pulse radiolysis. Aqueous solutions of the halocarbon and the biological compound (in the presence of isopropanol or tertiary butanol to increase solubility) are irradiated with a short pulse of electrons, usually in the nanosecond time region. The build up of the one electron oxidation product of the biological compound is monitored by kinetic absorption spectrophotometry. This buildup usually takes place in the microsecond time scale and precise rate constants for the reaction (3) can be evaluated.

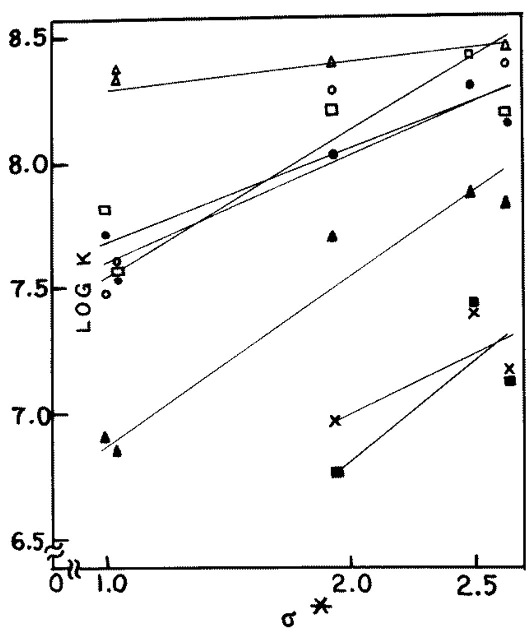

Figure 1. Correlation of log k for oxidation of tyrosine, xanthine, uric acid, guanine, hypoxanthine, and guanosine by various halogenated peroxyl radicals with the Taft's inductive parameter (σ^*) for these radicals: • xanthine; ⊔ guanine; × hypoxanthine; ∗ guanosine; ♢ tyrosine; ◯ uric acid (pH 6.8); and △ uric acid (pH) 12.6).

Table 1 below gives the bimolecular rate constants for various haloperoxyl radicals with a number of biological compounds, mostly purine type DNA bases [1]. The wide variation in the rate constants indicate that in living systems the behaviour of the parent halocarbon vary widely.

Quantitative analysis of these reactivities can be carried out by relating the inductive power of the halogen atoms in the halocarbon. This inductive power is given by the Taft's inductive parameter for the radicals.[1] Fig. 1 (taken from reference 1) shows the plot of the bimolecular rate constants against the Taft's parameter for the various radicals which shows a good linearity. Therefore perhaps one way of reducing the toxicity of these halocarbons is to use only those with low Taft's inductive parameters.

One other interesting fact we noticed was that carbon tetrafluoride CF_4 did not give rise to peroxyl radical oxidation products. This was because of the fact that electron addition does not break the carbon-fluorine bond, contrary to the carbon-chloride one. In the latter case, when an electron is added to the chlorine atom in a C-C bond, this bond breaks, giving a carbon centred radical and a chloride ion. The carbon centered radical adds an oxygen molecule, producing a toxic phenoxyl radical. This is one of the reasons why halocarbons containing only fluorine atoms are relatively less toxic and the chloro- fluorocarbons are the more toxic ones. In fact, ozone layer destroying chemicals, halocarbons containing only fluorine and no other halogens are very much safer. This is why they are being considered as substrates as refrigerants for present-day halocarbons.

The radiation chemistry of bilirubin

We have studied the reactions of various haloperoxyl radicals with bilirubin (BR) [the primary structure is given in Fig. 2], a product of heme catabolism and which is a very good hemoglobin model. The bimolecular rate constants show a linear relation with Taft's inductive parameter [2] just as in the case of purines.

[1] The Taft's inductive parameter is a measure of the electron withdrawing power of a substituent attached to a carbon atom. This is usually denoted by the symbol σ^*. This value is determined from the Hammet's equation and the values for a number of substituents are available in literature, see in 1. T. Taft, J. Am. Chem. Soc. 75 (1953) 4231 and 2. R. Taft, J. Chem. Phys. 26 (1957) 93.

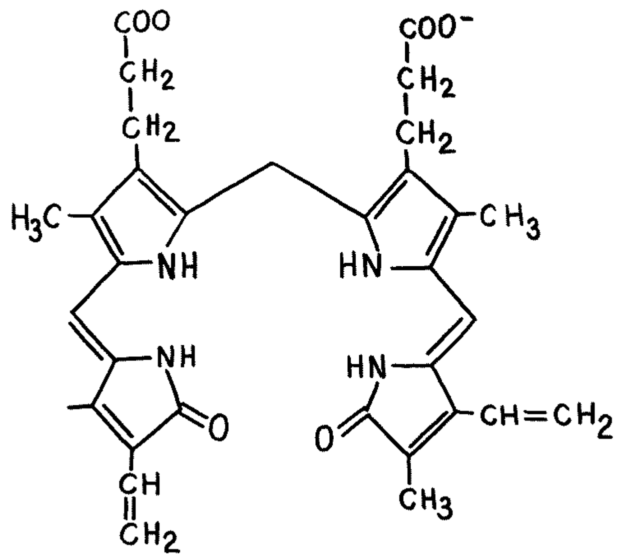

Figure 2. The primary structure of bilirubin (taken from ref 9)

More interesting work has been done, involving the study of radiation chemistry of BR in micellar system. In the human body BR is believed to act as an antioxidant protecting biomolecules from oxidative damage. However it is also known that micellar medium mimics biomembranes and globular proteins [3]. In homogeneous aqueous solution the radical $CO_2^{\cdot -}$ (produced by the reaction of $OH^{\cdot}$ radical with formate ion, the $OH^{\cdot}$ radical being produced pulse radiolytically) does not reduce BR. This radical is known to be present in living systems. However in micellar system we have shown that the radical $CO_2^{\cdot -}$ reduces BR [4]. Fig. 3 (taken from reference 4) shows the transient absorption spectrum for the reaction of $CO_2^{\cdot -}$ radical with BR in CTAB (acetyl trimethyl ammonium bromide) micellar medium. This reaction duplicates the reaction of BR in human intestines where it undergoes both oxidation and reduction reactions. This is another example where complex bioelectron transfer processes have been duplicated using pulse radiolysis techniques.

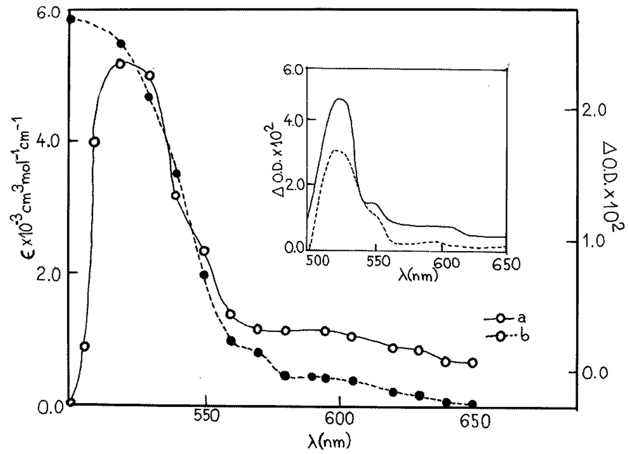

Figure 3. Transient absorption spectrum of the semireduced BR^{3-} radical produced in 1×10^{-4} mol dm^{-3} sodium formate in N_2 saturated aqueous solution of 2×10^{-2} mol dm^{-3} CTAB at pH 11: (a) uncorrected and (b) Corrected. Inset. Transient absorption spectra of semireduced BR recorded 100 μs after the e-pulse formed by the reaction of (—) e_{nq}^- and (***) $CO_2^{\cdot}$.

Charge transport in proteins and protein complexes

Using pulse radiolysis techniques it was found that in polypeptide or protein chains charge created by electron addition can travel as much as a few tenths of angstroms in micro second time scales [5,6]. Recently we have shown that positive charge transport can take place in the biological protein bovine serum albumin (BSA) [7]. Unfortunately the significance of these observations to molecular electronics in proteins has not still been adequately appreciated. Fig. 4 (taken from reference 7) shows the migration of positive charge in BSA after one electron oxidation by the radical anion $Br_2^{\cdot -}$. This radical was produced pulse radiolytically by the reaction of $OH^{\cdot}$ radical with Br^-.

$$OH^{\cdot} + Br^- \rightarrow Br^{\cdot} + OH^- \qquad (0.4)$$

$$Br + Br- \rightarrow Br_2^{\cdot -} \qquad (0.5)$$

It can be seen from Fig. 4 that the positive charge probably first produced on the sulfur-sulfur bonds of BSA and tyrosine moieties. In the subsequent $20\mu s$ the charge travels to the nearest tryptophan.

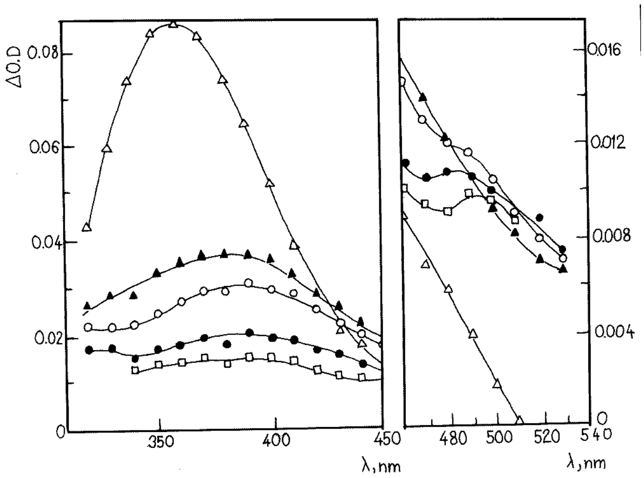

Figure 4. Pulse radiolysis (16 Gy per pulse) of N_2O saturated aqueous solution containing $5.0 \cdot 10^{-5}$ mol $\cdot$ dm_{-3} BSA, $1.0 \cdot 10^{-1}$ mol $\cdot$ dm^{-3} KBr at pH 6.9. Transient spectra are at △ 2 μs, ◇ 10 μs, ○ 20 μs, • 50 μs and ⊔ 80 μs after the pulse. Please note that from 460 nm onwards the y-axis is at R.H.S.

We believe that such transport process are due to the protein molecules acting as natural computers. Such processes may occur in the brain also with regard to storing of memories. It is known that there are two types of memories. These are respectively, short term and long term memories. We now know that long term memories are stored by the synthesis of new proteins. The mechanism for the storage of short term memory is not known. We suggest that these may be stored in the form of charges in proteins. Although this field merits further investigations, perhaps a few words are appropriate here to clarify some details.

Evidently, the life time of charge-carrying proteins should be correlated with the time scale of memory effects. At the same time, the reactions of the radiolytically produced free radicals will, of course, be over in microseconds and milliseconds. However, the charges created in protein molecules as a result of one electron oxidation or reduction can remain for a very long time. In fact, it has been shown in solid proteins that charge-carrying protein molecules can last for years. That memory is chemical reaction based and is now well accepted. We also know that many free radical oxidations and reductions occurring in living systems can be duplicated radiolytically. Therefore, our suggestion of charge based memory seems to be not speculative.

It is known that in the blood stream a number of biological molecules are carried by proteins in a complexed form. Very recently we have found that proteins protect these molecules from radical attack [8]. This supports our earlier suggestion that in living system proteins act as computers sensing the environment.

It would certainly be very interesting to correlate the life time of charge carrying protein molecules and the time scale of temporary memory. However, this would be a major effort needing collaborative work between neurologists, psychologists, biophysicists and chemists. Even modest progress in this direction would be regarded as a major leap in the status of our knowledge.

Our aim in writing the paper was much more modest. This was to bring to the attention of the readers the knowledge that has been created by the radiation chemists regarding proteins and how this lead to further work in which radiation chemists and Molecular Electronics/Biocomputing specialists can collaborate.

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SOME APPROACHES TO THE IMPLEMENTATION OF BIOMOLECULAR INFORMATION PROCESSING DEVICES

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INTRODUCTION: THE MAIN FEATURES OF THE BIOCOMPUTER MODELS USED

Approaches to the choice of the architecture for the biomolecular information processing devices capable of solving problems of high computational complexity were discussed earlier [1-4]. Proceeding from the results of this discussion let us deal with non discrete devices having massively parallel architecture and functioning on the basis of non-linear dynamic mechanisms. General theoretical features of this architecture were discussed in the previous papers [4-6].

The general scheme of a biomolecular device is shown in Fig. 1. The basic information processing operations of these devices are performed by a biomolecular dynamic media. It is complexity of the medium dynamics that determine the complexity of information processing operations performed by the medium.

We have made an attempt to investigate basic information processing capabilities of the simplest excitable biomolecular media having uniform spatial distribution of components. We choose Belousov-Zhabotinsky type media [7] as a model of a biomolecular excitable system. The dynamics of these media is similar to the dynamics of known biomolecular systems.

The dynamics of Belousov-Zhabotinsky type media are complex enough to demonstrate diverse and complicated behavior [7]. At the same time these media are stable, non-hostile reagents. Furthermore the temperature range and temporal operation scale of the medium dynamics are convenient for investigation with available physical methods.

The important feature of Belousov-Zhabotinsky media is that they can be considered as pseudo planar spatially uniform analogs of neural networks having lateral connections.

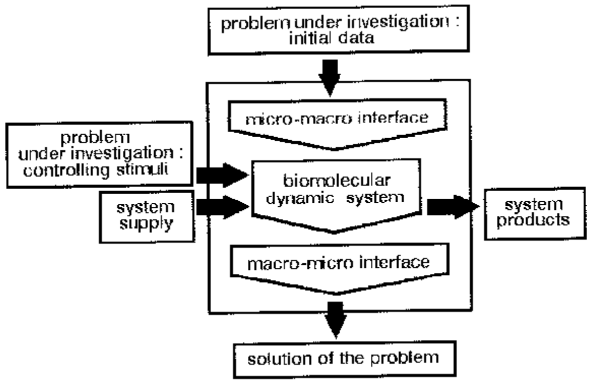

Figure 1. Schematic representation of the biomolecular information processing device based on non-linear dynamic mechanisms

It is possible to outline a number of structural features that would determine information processing characteristics of excitable media.

1. Small cells of an excitable medium compared in their dimensions with diffusion length can be considered as primitive processors representing chemical systems having point wise kinetics. If to consider these cells as independent, trigger and oscillatory regimes should be inherent in them. In common parlance, the diffusion length is a distance where total intermixing of reaction components takes place because of diffusion.
2. The coupling between cells is accomplished due to diffusion. It determines a number of complicated dynamic modes that are displayed in thin layers and in volume of excitable media.
3. The control of excitable medium regimes can be carried out by changing composition and temperature of the medium. One of the powerful variants of control can be based on the using of media containing light sensitive components. In this case the composition of the medium can be easily changed by light illumination. The degree of changes can be controlled by the light exposure.
4. Generally speaking due to diffusion coupling each cell is connected to each other cell of the medium. Nonetheless this interaction is carried out with a time delay proportional to the distance between cells and the strength of the interaction decreases proportionally to this distance.
5. The model representing a system of cells coupled by diffusion doesn't take into account that excitable media are uniform distributed systems. More adequate model should be invariant to infinitesimal shifts of the cell system along the surface of the medium.

Sufficient number of approaches to describe pseudo planar neural networks having lateral connections are known based on pioneer work by McCulloch and Pitts [8] in the long run. The comprehensive review of neural net models offered in 70's and 80's has been done by Grossberg [9].

The neural networks having image processing capabilities are discussed in this paper.

In the late sixties Pozin together with his coworkers performed a series of investigations summarized in the book [10].

The investigations of Pozin's group were based on neural net model represented a network having sigmoid feedback, containing both excitatory and inhibitory inputs. More exactly, the distribution of excitatory and inhibitory signals was set by individual coupling functions depending on distance between neurons in the network surface. The extended one or two-dimensional signals acting to neural network were considered. It was assumed that dimensions of input signal features are large compared with interneuron distances. Therefore neural networks were considered as continuous homogeneous media.

The main result obtained in the investigations [10] was that a signal input into neural network (for instance, a signal of rectangular distribution type) can be sharpened or broadened or a contour of the signal can be enhanced depending on a shape of the coupling function.

Later Yakhno with his collaborates (see, for instance, [11,12]) continued this line of investigations and used it for detailed analysis of image processing operations.

Beginning from the late sixties Grossberg launched detailed investigations of neural networks. During the last two decades Grossberg with his collaborates has analyzed different aspects of neural network activity. It is the image processing capabilities investigated by Grossberg et al [8,13-15] that are mentioned below.

Based on psychobiological and neurobiological data Grossberg concluded that shunting on-center off-surround feedback networks display a number of remarkable image features.

Grossberg has shown that shunting on-center off-surround feedback networks posses the key properties of:

1. solving the noise-saturation dilemma,
2. normalizing or conserving their total activity,
3. being capable of absolutely stable short-time memory.

These neural networks proved to be capable of quenching noises (sharpening) or amplifying noises (broadening) of input signals, or of enhancing its contour or the most intense fragments depending on the shape of neuron input function.

Grossberg [14] also has noted a dynamic analogy between shunting on-center off-surround feedback neural nets and reaction-diffusion systems which were used for the description of the process of biological pattern formation.

Later the analogy between the reaction-diffusion equations and the neural net integro-differential equations was showed by Masterov, Rabinovich, Tolkov, and Yakhno [16].

Thus different theoretical considerations show that the main information processing capabilities of neural networks should be first of all manifested in:

1. to store information in short-time memory,
2. to perform such operations as sharpening or broadening input signals, to enhance contour of an input picture.

EXPERIMENTAL

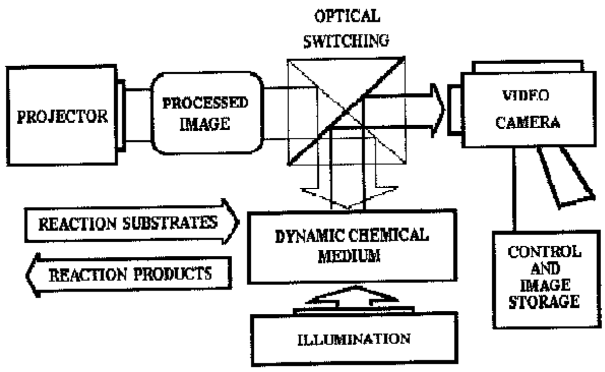

Figure 2. Schematic representation of the optical and digital video system for recording images produced by excitable media

The chemical dynamic processor was a thin (0.5-1.5 mm) flat non-stirred reagent layer placed in a siliconized dust-free reaction vessel in which spatio-temporal oscillating process proceeded. An excitation of a thin planar layer of the medium containing light-sensitive catalyst activated by light radiation was used for the input of information.

The optical and digital video system was used for detection of temporal evolution of the input image (Fig. 2).

The conditions of the experiment, and apparatus used were described in [17]. There are several dynamic modes inherent in Belousov-Zhabotinsky type processes [7].

The oscillating mode was chosen for the investigation of image processing by these media.

BASIC INFORMATION PROCESSING OPERATIONS OF DYNAMIC EXCITABLE MEDIA

The basic important feature of light-sensitive excitable media is that they store input information for a rather long period of time. Periodic processes of stored image transformation begin after projecting an image onto a thin layer of the medium.

It has been shown [18] that each period of these processes represents a combination of three interlaced primitive responses to the light excitation:

1. contour enhancement of image fragments,
2. alternation of negative and positive images of an input picture,
3. disappearance of small features of the picture.

The first of them predominates at relatively low medium acidity values and high exposures to light radiation. The second process appears at high acidity levels and low light exposures.

The responses of excitable medium to light excitation determine the character of primitive information processing operations that could be performed by the medium.

First let us discuss primitive information processing operations based on contour enhancement responses of an excitable media.

These operations can be divided into two main groups depending on the character of the image under processing.

The basic response of the medium (that is the enhancement of domains of sharp image brightness gradients) is one of the key image processing operation. In other words a picture could be divided into fragments as a result of this operation (Fig. 3B). Subsequently these fragments could be processed independently.

If a picture consist of one fragment this process is equivalent to contour enhancement of this fragment (Fig. 3A).

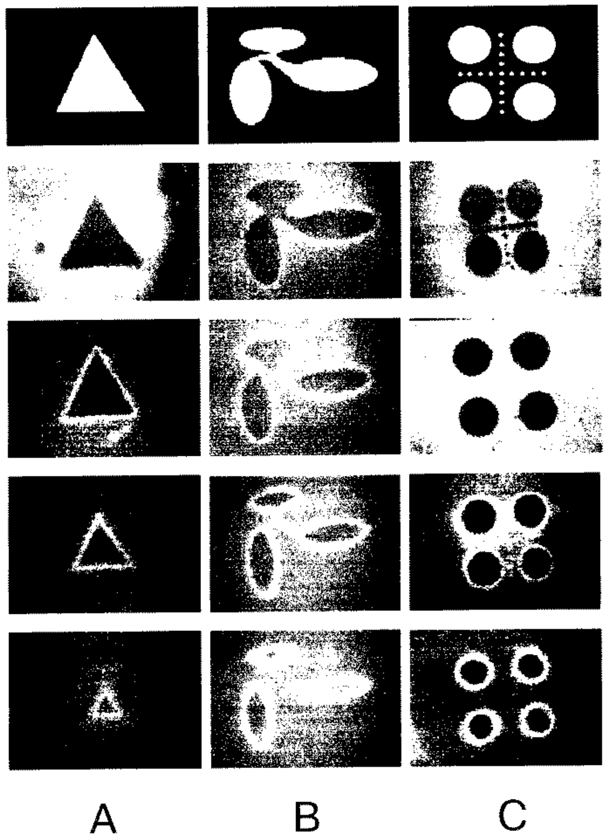

Figure 3. Responses of excitable media to the light excitation representing modes of: A - contour enhancement of an input image, B - segmentation of an input image, C - removing of small features of an input image

Here and in the next figure sequences show stages of the temporal evolution of the input image during one period of the oscillating process.

There are two ways of the following enhanced contour evolution.

1. If an original picture is a combination of white fragments placed on a black background the further movements of each fragment contours occur in the direction to their centers (Fig. 3A,B). In this case the evolution of the contour corresponding to the fragment having complex shape leads to the segmentation of the fragment. The result of this evolution represents the decomposition of the complex picture into its simple geometrical components (Fig. 3B).

   In the course of further evolution contours of each simple part are transformed into their geometrical centers or into their skeletons.

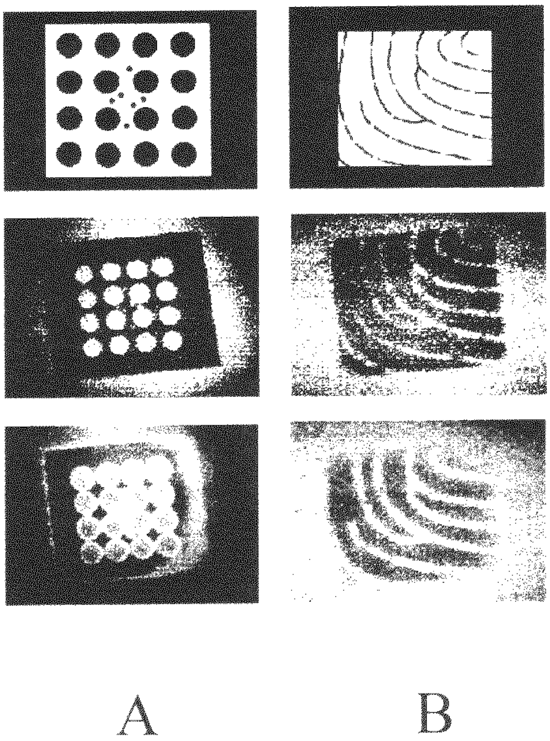

Figure 4. **Responses of excitable media to the light excitation representing modes of: A - accentuation of small features of an input image, B - restoration of the spoiled image**

2. If an original picture represents a combination of black fragments on the white background contours of its fragments move in directions opposite to their centers. In this case the evolution of an image leads, as if were, to the synthesis of a new picture. Some opportunities to use this process for the image processing are of a great interest.

   Some versions of this process can be considered as 'addition to the whole' operations. For instance, the restoration of the image takes place if the lost parts are not very large.

   The restoration of artificially constructed (but damaged) fingerprints is shown in Fig. 4B, as an example of this process.

   Different input modes (white fragments on the black background or vice versa) can be used for the implementation of another useful image processing operation.

   The removing of small parts of the picture take place if the picture represents white fragments on the black background (Fig. 3C). Processes of this type are equivalent to random noise filtering if the dimension of removed fragment is not too large.

   If a picture consists of black fragments on the white background accentuation of small features of the picture take place. This process is shown in Fig. 4A.

   The image processing operations performed by excitable media was considered in details elsewhere [19].

DISCUSSION

Given experimental results discussed in the previous sections of the paper, it is possible to conclude that the main information processing features of biomolecular excitable media are similar to these features of neural networks described by different theoretical models.

First of all excitable media are capable of short-term memory. As mentioned above an input image is stored by the medium for a rather long period of time subjecting to the process of image transformation.

In the course of the basic periodic process the evolution of an image stored by the excitable medium looks as if it is subjected more and more to the action of a blur filter at each period of the basic process. The half width of the extracted contour increases gradually from one period of the basic process to another.

The duration of the basic process during which an image remains sufficiently clear ranges from ten (about five minutes) to several tens (up to one hour or more) of periods, depending on the state of the medium and the contrast of the initial image.

It was shown that excitable media are capable of quenching or amplifying small features (noises) of the input image depending on the state of the medium and the character of the input image. Important dynamic feature is also the contour enhancement of the input picture.

It should be noted that these processes of the temporal image evolution can be rather successfully described by the solutions of reaction-diffusion equations. For instance, the process of the contour enhancement and some other features were calculated by Balkarey, Evtichov, and Elinson [20]. The amplifying of small features and spoiled image restoration were demonstrated by Price, Wambacq, and Oosterlinck [21].

Therefore it is possible to conclude, given the analogy between neural networks and reaction-diffusion systems, that the more sophisticated neural network models seem to be capable of describing in more details experimental dynamics of excitable media.

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QUANTUM MECHANICAL DESIGN OF BASIC ELEMENTS OF MOLECULAR COMPUTERS

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1. INTRODUCTION

Synthesis and construction of truly unimolecular devices [1-6] which focuses on the properties of a single organic or biological molecule is in the initial stage now.

Investigation of basic elements for molecular neural networks is one of evolving area of neuromolecular computing science [7-9]. Networks constructed from nanoscale elements - organic molecules have advantage over silicon based networks [10] in their speed and learning capabilities. The projects of molecular shift register memory based on photoinduced electron transfer phenomenon in organic supermolecules [11], molecular organic cellular automaton based on phthalocyanine molecules [12], molecular electronic NAND gate [13, 14] and self-assembly computer based on fullerene C_{60} molecule dimmers [15] were proposed.

2. THE REVUE OF RESEARCH IN THE FIELD OF MOLECULAR ELECTRONICS HAVE BEEN PERFORMED IN LITHUANIA

The idea of quantum mechanical investigation and fabrication of nanosize devices and biological computers made from biological molecules in Lithuania was encouraged by academician Adolfas Jucys (12 September 1904–04 February 1974) early in seventies.

The term "molecular electronics" at first in Lithuania have been used in laboratory of prof. L. Valkunas in eighties. The origin of photosynthesis in the molecular derivatives level was investigated in this laboratory at that time and continue now. The first Lithuanian papers in the field of molecular electronics [16] were published in second symposium on "Molecular Electronics and Biocomputing". At that time Dr. J. Alekna have produced and investigated Langmuir-Blodgett films in the Semiconductor Physics Institute and Dr. V.I Silin, Dr. V.-R. Talienė have produced and investigated thin artificial enzyme layers in Institute of Biochemistry. There is still a high quality laboratory of organic synthesis in the faculty of chemistry of Vilnius University under the guidance of Dr. P. Adomėnas.

Some research during last five years have performed in our theoretical molecular electronics laboratory are as follows.

The quantum chemical calculations and investigations of three photo electron donor molecules: carbazole (abbreviation of this compound will be Cz and formula is $C_{12}H_9$N), N,N,N',N'-tetramethyl-1,4-phenylenediamine (abbreviation: TeMePhDA, formula: $C_6H_4[N(CH_3)_2]_2$), 1,4- phenylenediamine (PhDA, $C_6H_4(NH_2)_2$); several organic electron acceptor molecules: 2,4,7-trinitro-9-fluorenone (TNF, $C_{12}H_5O(NO_2)_3$), 2,4,5,7-tetranitro-9- fluorenone (TeNF, $C_{12}H_4O(NO_2)_4$), 7,7,8,8- tetracyanoquinodimethane (TCNQ, $C_8H_4(CN)_4$), 2,4,7-trinitro-9-dicyanofluorene (TN9$(CN)_2$F, $C_{12}H_5C(CN)_2(NO_2)_3$), 2,4,5,7-tetranitro-9-dicyano-fluorene (TeN9$(CN)_2$F, $C_{12}H_4C(CN)_2(NO_2)_4$), 1,2,4,5-tetracyano- benzene (TCNB, $C_6H_2(CN)_4$), 2,3,5,6-tetrachlor-1,4- benzoquinone (TeClBQ, $C_6Cl_4O_2$), 2,3,5,6-tetrafluoro-7,7,8,8-tetracyanoquinodimethane (TeFTCNQ, $C_8F_4(CN)_4$) and others; palmitic acid molecule (CH_3-(CH_2)$_{14}$-COOH); carbazole-containing supermolecules (carbazole is connected via the alkane or alkene electron insulator bridges with electron acceptor molecules) and carbazole-containing supramolecules (carbazole and electron acceptor molecules are stabilized by the van der Waals forces) were performed [17-23] using semiempirical MNDO, AM1, PM3 [24, 25] and CNDO/S-CI methods [26]. The results of our investigations show that photoactive charge transfer carbazole- containing supermolecules and supramolecules should be molecular implementation of photodiodes [18, 20-23].

Taking into account 120 single excited configurations, calculations of singlet state bands of two C_{60} molecules in softer region are in good agreement with experimental values of absorption spectrum of C_{60} clusters in water solution or in the Langmuir-Blodgett films. The CNDO/S-CI calculation results show three new additional bands in the regions 342.90-364.46 nm, 427.28-437.08 nm and 481.58-495.88 nm [27]. Quantum chemical investigations of a charge transfer singlet state band of the proposed system consisting of two C_{60} molecules and two small charges are performed in the framework of CNDO/S-CI method taking into account 60 single excited configurations. Results of calculations show the existence of a charge transfer band in this system of two C_{60} molecules [27]. This enables to design unimolecular and bulk photoactive molecular devices based on charge transfer process. The projects of photodiodes and radiation solar energy conversion cells based on photoactive polymers and C_{60} layer or other C_{20+2n} molecular films are proposed [28]. Calculated small values of ionization potentials of endohedral metallofullerenes show possibility to employ photoinduced charge transfer process in various molecular electronics devices. Possible solar energy conversion cells are based on heterojunctions: metallofullerene Me@C_{60} molecules layer/fullerene C_{60} molecules layer and similar heterojunctions with metallofullerene Me@C_{20+2n} molecules [28]. The proposed molecular implementation of cellular automata are based on two phenomena: 1) changes of singlet spectrum of two C_{60} molecules in their mutual rotation and 2) photoactive charge transfer in endohedral fullerene A@C_{60} molecules [28].

Quantum mechanical investigations of stability of empty fullerene C_{20+2n} $(n = 0, 2, 3, \ldots, 16, 20)$ molecule isomers with highest symmetry and the same cage endohedral fullerenes with twenty eight encapsulated even valence atoms: Be C, O, Mg, Al, Si, S, Zn, Ge, Se, Cd, Sn, Te, Hg, Pb or odd valence atoms: H, N, F, P, Cl, Ga, As, Br, In, Sb, Tl, Bi were performed using point set group theory in the framework of semiempirical MOPAC-PM3 method [24, 25]. The main criterion of stability of calculated empty or endohedral fullerene molecules we state that their highest occupied molecular orbital (HOMO) must be completely electron filled - without free valences. We have found that empty C_{24}, C_{26}, C_{32}, (isomer with D_{3d} symmetry), C_{34} (C_{3v}), C_{36} (D_{6h}), C_{42} (D_3), C_{44} (T), C_{46} (C_3), C_{48} (D_{6d}), C_{50} (D_{5h}) molecules are stable. We state also that completely filled HOMO endohedral fullerene molecules which posses positive energy of formation (i.e. difference between total energy of endohedral fullerene molecule and the sum of total energies of corresponding empty fullerene molecule and encapsulated atom) must be most stable. We are using for the evaluation of stability of endohedral fullerenes from the energetic point of view such a formula:

$$\Delta E = \mid E_{tot}(A@C_{20+2n}) \mid - \mid E_{tot}(C_{20+2n}) + E_{tot}(A) \mid, \tag{0.6}$$

where $E_{tot}(\mathrm{A}@C_{20+2n})$ is the total energy of certain endohedral molecule ($n = 0, 2, 3, \ldots, 16, 20$), $E_{tot}(C_{20+2n})$ - total energy of certain empty fullerene molecule and $E_{tot}(\mathrm{A})$ - total energy of certain encapsulated atom. We state that fullerene should be more stable in the case if energy of formation (ΔE) is positive and metastable - if ΔE is negative.

The completely filled HOMO endohedral fullerene molecules which posses positive energy of formation are: Be@C_{24}, Ga@C_{24}, Be@C_{34}, In@C_{34}, Si@C_{34}, Ge@C_{34}, H@C_{36}, Be@C_{36}, Al@C_{36}, Ga@C_{36}, Si@C_{36}, Se@C_{36}, Te@C_{36}, Ge@C_{40}, Se@C_{40}, Te@C_{40}, H@C_{42}, Ga@C_{42}, In@C_{42}, Si@C_{42}, Se@C_{42}, Te@C_{42}, H@C_{44}, Se@C_{46}, Te@C_{46}, Si@C_{48}, Ge@C_{48}, Se@C_{48}, Te@C_{48}, H@C_{50}, Si@C_{50}, Se@C_{50}, Te@C_{50}, Se@C_{52}, and Te@C_{52}. Several metastable endohedral fullerene molecules after additional optimization of geometry becomes as stable. They are: Si@C_{30}, Si@C_{32}, Br@C_{36}, Ge@C_{42}. 106 completely filled HOMO endohedral fullerene molecules which posses negative energy of formation we have found to be metastable.

The process of reducing of highest symmetry conformers of fullerene molecules C_{28}, C_{26} and C_{24} due to the effect of H.A. Jahn - E. Teller was investigated. Occurs that conformer with highest symmetry (D_{6h}) of empty molecule C_{24} is not stable. The most stable is conformer with D_6 symmetry and conformation ${}^1A_1$ [29]. Investigations were performed in the framework of MOPAC-PM3 configuration interaction method.

We propose to use endohedral atoms of stable and metastable endohedral fullerene molecules for the construction of quantum gates - the same as was done with atoms in cavities [30] and trapped ions [31].

Quantum chemical calculations of pentayne, electron acceptor molecules and supramolecules are performed by using the program MOPAC in the framework of semiempirical PM3 method [24, 25]. We have used the PM3 method in this work because it is better for the calculations of supramolecules in comparison with the MNDO method used in the calculations of the carbazole-containing supramolecules [18, 20-23].

We have found the geometries of pentayne, electron acceptor molecules and supramolecules with MOPAC-PM3 programme. We used MOPAC capability to keep some dependencies of geometry variables during optimization. We changed the coordinates x, y, z and the torsional angle between two molecules in supramolecules during the optimization.

For the evaluation of stability of supramolecules we are using a formula from the energetic point of view:

$$D = \mid E_{tot}(supramol) \mid - \mid E_{tot}(pent) + E_{tot}(accept) \mid \quad (0.7)$$

where D is the energy of formation of the supramolecule, E_{tot}(supramol) is the total energy of certain supramolecule, E_{tot}(pent) - total energy of certain pentayne molecule and E_{tot}(accept) - total energy of certain electron acceptor molecule. We state that the supramolecule should be stable if the energy of formation is positive, and unstable if D is negative. The stability is ranked according to the value of D.

The ionization potentials and dipole moments of four disc-like pentayne (pentakis(phenyle thynyl)phenyl) molecules with radicals R= $-OC_5H_{11}$, $-CH_3$, $-CF_3$ and -CN were calculated using the MOPAC-PM3 method. All pentayne molecules are photo-induced electron donors (ionization potentials were evaluated by using Koopman's approximation). The best photo electron donor should be pentayne with radical $-CH_3$ ($I_p = -8.47eV$). All pentayne molecules possess dipole moments.

The electron affinity and dipole moments of seven organic electron acceptor molecules: TNF, TeNF, TCNQ, TN9$(CN)_2$F, TCNB, TeClBQ, TeFTCNQ were calculated using the MOPAC-PM3 method. Results of our calculations show that all these molecules are electron acceptors (electron affinities were evaluated by Koopman's approximation). The best electron acceptors should be TeFTCNQ and TeNF ($A_f = -3.62eV$ and $-3.38eV$ respectively). TNF, TeNF and TN9$(CN)_2$F molecules possess dipole moments.

The quantum chemical calculations and investigations of the stability of twenty eight photoactive charge transfer supramolecules constructed from disc-like pentayne (pentakis(phenyle thynyl)phenyl) molecules with radicals R = $-OC_5H_{11}$, $-CH_3$, $-CF_3$ and -CN and seven organic electron acceptor molecules: TNF, TeNF, TCNQ, TN9$(CN)_2$F, TCNB, TeClBQ, TeFTCNQ were performed using MOPAC-PM3 method.

All supramolecules have relatively small energetic gap, i. e. they are good electron donors and at the same time good electron acceptors. Therefore these supramolecules should be suitable for the molecular implementation of photodiodes.

Energies of formation (D) are largest for supramolecules constructed from disc-like pentayne with $-CH_3$ radical and TeNF or TN9$(CN)_2$F molecules - 2.16 kcal/mol and 2.20 kcal/mol respectively. The order of decreasing our calculated stability of supramolecules with various radicals is: $-CH_3 > -OC_5H_{11} > -CF_3 > -CN$. It should be explained that because the $-CH_3$ and $-OC_5H_{11}$ groups are relatively inertial and do not interact strongly with electron acceptor molecules. Electron acceptor groups $-CF_3$, -CN are much more active and repulse acceptor molecules. The most stable supramolecules are with electron acceptor molecules TeNF and TN9$(CN)_2$F. The above mentioned electron acceptor molecules possess the largest dipole moments, and induce additional dipole moments in the disc-like pentayne molecules. Experimentally confirmed existence of stable supramolecule: cyano-pentayne::TNF [32]. The order of decreasing our calculated stability of supramolecules with various electron acceptor molecules is: $TN9(CN)_2F > TeNF > TNF > TeFTCNQ > TCNQ > TCNB > TeClBQ$. The optimization of intermolecular orientation and distances in supramolecules were done. The distances between planes in the supramolecules calculated in the framework of MOPAC-PM3 are in the region $4.38\mathring{A} - 5.15\mathring{A}$ i.e. smaller than during the calculations of carbazole-containing supramolecules performed by the method MNDO ($5.1\mathring{A} - 5.3\mathring{A}$) [18, 20-23]. Our new results show better agreement with the experimental intermolecular distances in supramolecules.

Electron charge redistribution exists in supramolecules. The negative charge in the pentayne molecules flows towards the site which is the projection of the electron acceptor molecule. Therefore all electron acceptor and pentayne molecules in the supramolecules possess induced local dipole moments. All the supramolecules possess the dipole moments. The acceptor groups of pentaynes $-CF_3$, -CN repulse active groups of acceptor molecules - it makes influence on the intermolecular orientation of molecules in supramolecules.

Molecules TeNF, TN9$(CN)_2F$ and TNF are oriented approximately the same way in the supramolecules with pentayne molecules which possess radicals $-CH_3$ and $-OC_5H_{11}$. It is due to the interaction of the $-CH_3$ and $-OC_5H_{11}$ groups with the electron acceptor group $-NO_2$. The $-CF_3$ and -CN groups on the pentayne molecules are negatively charged. Therefore electron acceptor molecules TN9$(CN)_2$F and TNF are oriented approximately the same way in the supramolecules with pentayne molecules which possess radicals $-CF_3$ and -CN. The molecules TCNQ and TeFTCNQ are oriented approximately the same way in the supramolecules with pentayne molecules which possess radicals $-CH_3$ and -CN. The molecule TeClBQ is oriented approximately the same way in the supramolecules with pentayne molecules which possess radicals $-CH_3$ and $-CF_3$. It is because the $-CF_3$ and -CN fragments are negatively charged. The strongest interactions occurs in supramolecules: TNF::pentayne-OC_5H_{11}, TeClBQ::pentayne-OC_5H_{11}, TNF::pentayne$-CH_3$, TeN9$(CN)_2$F::pentayne$-CH_3$, TeNF::pentayne$-CH_3$. Usually the out of plane atoms and moieties of the molecules are responsible for the largest values of intermolecular bond orders (they are approximately in order 10^{-4} - 10^{-6}), i.e. self-assembly and formation of appropriate supramolecules.

Conclusions of the investigations of disc-like supramolecules:

1. All investigated supramolecules: disc-like pentayne molecules::electron acceptor molecules are stable, possess dipole moments and are potential molecular photodiodes.
2. The order of decreasing calculated stability of the above mentioned supramolecules with various radicals is: $-CH_3 > -OC_5H_{11} > -CF_3 > -CN$.
3. The order of decreasing calculated stability of investigated supramolecules with various electron acceptor molecules is: $TeN9(CN)_2F > TeNF > TNF > TeFTCNQ > TCNQ > TCNB > TeClBQ$. The research of series disc-like pentayne supramolecules was done with J. Tamulienė and E. Stumbrys (Vilnius University, Faculty of Physics).

3. DESIGN OF BASIC ELEMENTS OF DIGITAL MOLECULAR COMPUTERS

Some preliminary results of our design of molecular implementation (MI) of basic elements of digital and post-digital computers have been published [28], reported in conferences [33, 34] and sent to the journals [35, 36]. They are as follows.

Molecular implementation of two, three, four variable logic functions, summators of neuromolecular networks and cells of quantum cellular automata are designed based on results of quantum chemical calculations of photo electron donor, electron insulator, elecron acceptor, fullerene C_{60}, $C_{28}H_4$ $C_{20}H_6$ and endohedral fullerene A@C_{60} molecules. Complete set of sixteen molecular implementation of two variable logic functions (for example OR, AND, Implication, Equivalence, Difference etc.) is designed and also proposed using molecular implementation of two variable molecular logic function initial basic sets: {OR, AND, Negation} or {NOR}, or/and {NAND}.

We will describe in more detail in this article the design of two variable logic functions OR, NOR, AND and NAND molecular implementation using organic planar PhDA, TeMePhDA, TeClBQ, TCNQ molecules. These MI two variable logic functions can compose the initial sets of a complete set of sixteen MI two variable logic functions.

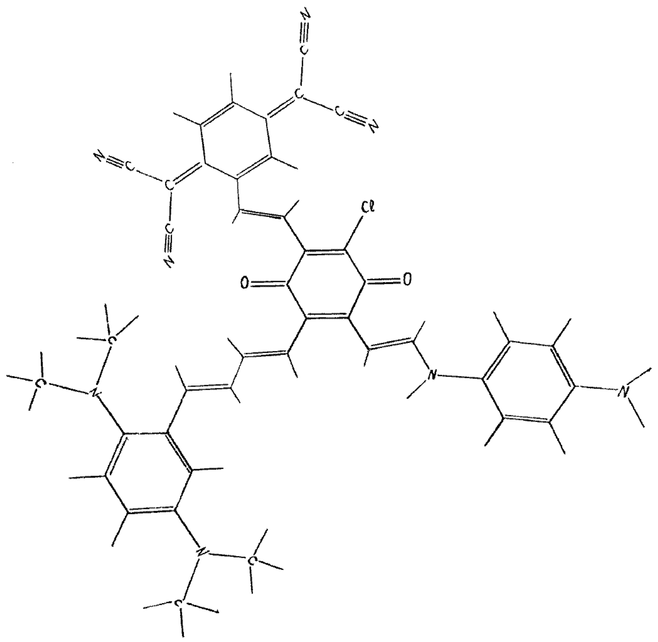

Figure 1.

3.1. Molecular implementation of disjunction (OR) and NOR logic functions

Two various MI disjunctions and MI NOR were designed: 1) from planar PhDA, TeMePhDA, TeClBQ, TCNQ molecules (see Fig. 1) and 2) from PhDA, carbazole and fullerene C_{60}, $C_{28}H_4$ molecules (see [35]).

Two photoelectron donor molecules: PhDA and TeMePhDA (two inputs of this logic gate which it is possible in principle to excite by two different wavelengths) are connected via an electron insulator bridges -C_2H_2- and -C_4H_4- respectively with the fragment of electron acceptor molecule TeClBQ and further via the electron insulator bridge -C_2H_2- with the second electron acceptor molecule TCNQ - output of this logic gate (see Fig. 1). The present state of experimental physics allow to measure single electron charge [37-39] therefore in principle it possible to measure the additional electron charge on single electron acceptor TCNQ molecule in ground state.

Let us imagine that we do not excite by light no one photo electron donor molecule (not send signals on the input) of this MI OR gate. Then we do not measure the additional electron charge on the TCNQ molecule (on the output of this gate) - we should have response 0. In the case if we should excite by light one photo electron donor molecule (one of two inputs) electron should jump from photo electron donor molecule to the fragment of TeClBQ molecule and we should measure the additional electron charge on TCNQ molecule (because according to our calculations TeClBQ molecule is worse electron acceptor than TCNQ and electron hopping from fragment of TeClBQ molecule to TCNQ molecule should exists). Therefore we should have responses 1 on the output of the gate in both cases: if excite PhDA or TeMePhDA molecule. In the case if we excite both photo electron donor molecules PhDA and TeMePhDA on the input of the gate at the same time we should measure additional electron on the TCNQ molecule as well - we should have response 1 on the output of the gate. Summarizing in all four possible input cases of this two variable logic gate we should have sequence of responses on the output - TCNQ molecule: 0, 1, 1, 1. It means that this our MI logic function is disjunction.

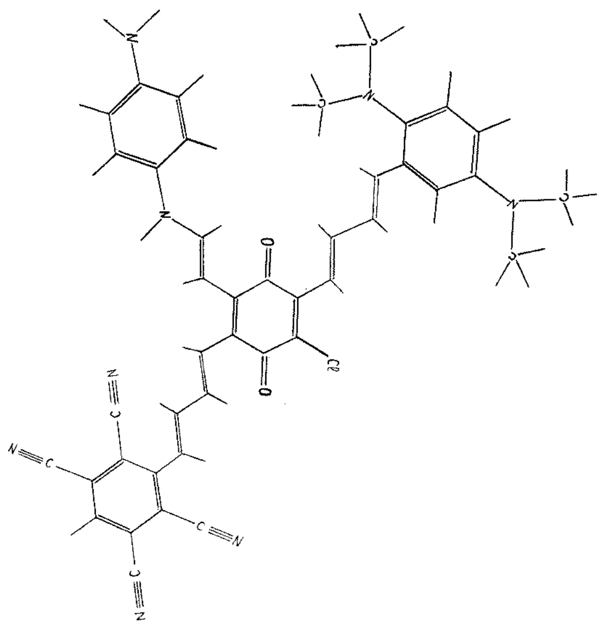

Figure 2.

We should have MI logic function NOR in the same device in the case if we excite PhDA or/and TeMePhDA molecules on the input of the same gate but measure on the output spectrum of the neutral (without additional electron charge) TCNQ molecule because we should have sequence of responses on the output - TCNQ molecule: 1, 0, 0, 0.

3.2. Molecular implementation of conjunction (AND) and NAND logic functions

Two various MI conjunctions and MI NAND are designed: 1) from planar PhDA, TeMePhDA, TeClBQ, TCNB molecules (see Fig. 2) and 2) from PhDA, carbazole, empty fullerene C_{60} and endohedral metallofullerene Me@C_{60} molecules (see [35]).

Two photo electron donor molecules: PhDA, TeMePhDA (two inputs of this gate) are connected via electron insulator bridges -C_2H_2- and -C_4H_4- with the fragment of electron acceptor molecule TeClBQ and further via the bridge -C_4H_4- with the second electron acceptor molecule TCNB - output (see Fig. 2). Let us imagine that we measure additional electron charge in the ground state TCNB molecule. In the case if we should not excite no one of two photo electron donor molecules on the input of this gate we should not measure the additional electron charge on the output - TCNB molecule. Therefore in this case we should have response on the output: 0. In the case if we should excite by light one of two photo electron donor molecules we also should not measure the additional electron charge on the output of this gate - TCNB molecule (because according to our calculations TeClBQ molecule is better electron acceptor than TCNB and electron hopping from the fragment of TeClBQ molecule to TCNB molecule should not exists). Therefore in all these two cases we should have responses on the output: 0. In the case if we should excite at the same time both photo electron donor molecules (two inputs) we should measure electron on the output - TCNB molecule because one additional electron prefer to jump from twice charged fragment of TeClBQ molecule to TCNB molecule. Therefore we should have response on the output: 1. Summarizing in all four different cases of this two variable logic gate we should have sequence of responses on output - TCNB molecule: 0, 0, 0, 1. It means that this our MI logic function is conjunction.

We should have MI logic function NAND in the same device in the case if we excite PhDA or/and TeMePhDA molecules on the input of the same gate but measure on the output spectrum of neutral (without additional electron charge) TCNB molecule because we should have sequence of responses on output - TCNB molecule: 1, 1, 1, 0.

4. DESIGN OF BASIC ELEMENTS OF POST-DIGITAL MOLECULAR COMPUTERS

Molecular implementation of five cells of molecular cellular automata and three summators of neuromolecular networks and are designed using results of quantum chemistry calculations of electron acceptor, photo electron donor and electron insulator molecules, carbazole-containing oligomers, supermolecules, supramolecules, empty fullerene molecules: C_{60}, $C_{28}H_4$, $C_{20}H_6$ and endohedral fullerene molecules A@C_{60} [28, 33, 34].

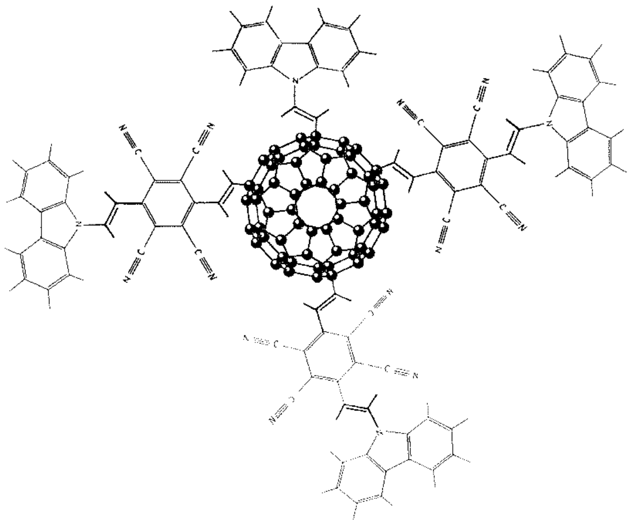

Figure 3.

The molecular cell simulating one of Life figures is presented in Fig. 3. This molecular cell satisfy such conditions: 1) if three neighbors (photoactive Cz molecules) are excited by light then central cell (C_{60} molecule) which is connected with Cz molecule via electron acceptor molecules TCNB and/or electron insulator bridges -C_2H_2- becomes excited (posses additional electron charge), 2) if central cell initially was excited and one or two neighbors are excited then central cell continues to be excited, 3) if initially central cell was excited and four neighbors are excited then central cell lose excitation.

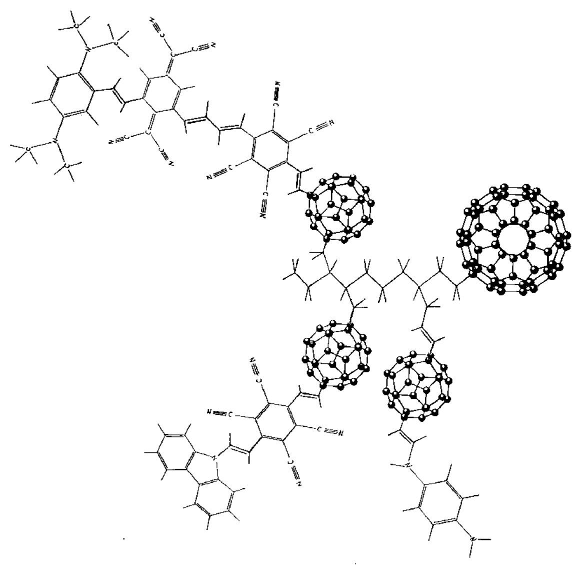

Figure 4.

One of summators of neuromolecular networks (see Fig. 4) is designed from three different variable resistors with inputs of three different photo electron donor molecules: Cz, PhDA and TeMePhDA, electron acceptor molecules: TCNQ, TCNB and fullerene $C_{28}H_4$, electron insulator bridges: $-CH_2$-, -C_2H_2-, -C_4H_4- and CH_3-$(CH_2)_9$- and output of C_{60} molecule. This summator should simulate sigmoidal behavior of artificial neuron.

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SELF-ASSEMBLED LIPID BILAYERS ON SOLID SUPPORT AS A SMART MATERIAL FOR NANOTECHNOLOGY

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ABSTRACT

Biological membranes play a crucial role in energy conversion, information processing and signal transduction. This is owing to the fact that most physiological activities involve some sort of lipid bilayer-based receptor-ligand contact interaction. There are many outstanding

examples such as ATP synthesis, ion sensing, antigen-antibody binding, and ligand-gated channels, to name a few. One approach to study these interactions in vitro is facilitated by employing artificial bilayer lipid membranes(BLMs). Our current efforts have been focused on ion and/or molecular selectivity and specificity using recently available self-assembled BLMs on solid support (i.e. s-BLMs) which, with their enhanced stability, greatly aid in research areas of membrane biochemistry, biophysics, and cell biology as well as in biosensor designs and molecular devices development. In this report, our current work along with the experiments done in collaboration with others on s-BLMs will be presented.

INTRODUCTION

In the past few years there have been a number of reports on self-assemblies of molecules as 'advanced materials' or 'smart materials'. Without question, the inspiration for this exciting work comes from the biological world, where, for example, the lipid bilayer of cell membranes plays a pivotal role [1,4,8,12.25.26]. The seminal work on the self-assembly of lipid bilayers (bimolecular lipid membranes, or BLMs for short) was carried out by Rudin and his colleagues in 1959-1960 [1,4]. Since the mid 1960s, our work has been motivated by the desire to explain the living system in physical, chemical and physiological terms. The area chosen for investigation is membrane biophysics, where the cell membrane plays a crucial role in the signal transduction, energy conversion and information processing. This is owing to the fact that most physiological activities involve some kind of lipid bilayer-based ligand-receptor contact interactions. Outstanding examples among these are ion sensing, antigen/antibody binding, light conversion and detection, and gated channels, to name a few. The conventional BLM system has one major drawback in that it is notoriously unstable, rarely lasting more than a few hours. As a result, many attempts have been made to stabilize this extremely delicate lipid bilayer structure for fundamental studies and practical applications. In this connection, a report was published in 1978 describing the formation of supported BLMs in polycarbonate filters with much improved stability to both chemical and mechanical disturbances[2]. Our present approach to study these interactions is facilitated by employing self-assembled bilayer lipid membranes on solid support (s–BLMs) [3-5,10]. Presently, our efforts have been focused on ion and/or molecular selectivity using the s-BLM system whose enhanced stability greatly aids in research areas of membrane biophysics, biochemistry and molecular cell biology as well as in biosensor designs and molecular devices development. It should be noted that the dimensions of a typical s-BLM under investigation is about $2 \times 10^{-5} cm^2$ in area and $5nm$ in thickness. This new type of s-BLM-based probes is destined for microelectronic fabrication. In this paper, a brief description of the new s-BLM system on solid support will be given. This will be followed by a review of our recent work together with current considerations of s-BLM-based molecular technologies.

THE s-BLM SYSTEMS

Preparation and Characterization of Solid Supported BLMs

Bilayer lipid membranes (or lipid bilayers) on solid support (i.e., s-BLMs) have been formed by a number of methods including the two/consecutive step technique as follows: Step (i) placing a Teflon- coated metal wire (e.g., Pt, stainless steel or Ag) to be cut in contact with a BLM-forming lipid solution and then cut it with a sharp knife and, Step (ii) immersing the lipid layer that has adsorbed onto the metal wire surface into an aqueous solution. For the best cutting of metal wires, a miniature guillotine has been used, where the sharp knife is moved vertically onto the wire placed on a flat surface and immersed in a lipid solution (see Ref. 5 for a summary of the s-BLM techniques). Typically we used either a 1% glycerol dioleate in squalene or 1% phospholipid (lecithin) in n-decane. Into these s-BLMs, three classes of compounds have been embedded [1,7,8]: (a) Electron acceptors, donors, and mediators including highly conjugated compounds such as meso-tetraphenylporphyrins (TPP), metallo-phtalocyanines (PLC), TCNQ (tetracyano-q-quinodimethane), TTF (tetrathiafulvalene); (b) Redox proteins and metalloproteins such as cytochrome c, and iron-sulfur proteins (ferredoxins and thioredoxins). Specifically, the ligand may be a substrate, an antigen, a hormone, ions, or electron acceptor or donor, and the corresponding receptor embedded is s-BLM may be an enzyme, an antibody, a protein complex, a carrier, a channel, or a redox species; and (c) Fine semiconductor particles (formed *in situ*) such as CdS, CdSe, and AgCl. We have worked with some of these compounds in the past in conjunction with conventional BLMs [6-8]. Hence, methodologies developed for *in situ* formation of semiconductor particles on conventional BLMs will be applied to s-BLM systems.

Formation of Gel Supported BLMs

Techniques are also available to form planar BLMs on gels [9,10]. The formation procedure consists of three steps. In the first step, a chlorided Ag wire (Ag/AgCl) is inserted into a Teflon tubing which has been previously filled with a mixture of agar or agarose and KCl solution saturated with AgCl. The AgCl electrode and the filled Teflon tubing are glued together with wax at the point of insertion. In this way an Ag/AgCl-Teflon salt bridge is constructed. In the second step, the tip of the other end of the Teflon salt bridge is cut in situ while immersed in a BLM-forming solution with a scalpel. In the third and last step, the Ag/AgCl-Teflon salt bridge with freshly lipid solution coated tip is immersed in $0.1M$ KCl solution of the cell chamber. Alternatively, the second step described above may be carried out in air and then immediately immersed the freshly cut end of the salt bridge in the lipid solution for a few minutes. In either case, the cell chamber filled with an appropriate aqueous solution (e.g., $0.1M$ KCl) contained an Ag/AgCl reference electrode and an Ag/AgCl-Teflon salt bridge with a self-assembled BLM at its end. The lead wires of the two electrodes are connected to the measuring instrumentation. Further details may be found in the cited references [5,9]. More recently, we have studied the effect of trehalose and glucose on the stability of s-BLMs [22]. Interestingly, treatment of s-BLM in electrolyte containing $300mM$ trehalose permitted s-BLMs to be stored dry in refrigerator for several days without altering the membrane parameters. The stabilizing effect of polysaccharides on BLMs was also observed earlier [19].

Electrical Measurements

In voltammetry the potential of the cell is varied and the corresponding current is monitored. One type of voltammetry is called cyclic voltammetry and employs a triangular voltage waveform. The graph with the current plotted on the vertical axis vs. the potential on the horizontal axis is called the voltammogram, which is characterized by several parameters. The working electrode (WE) may be made of Pt, Au, or carbon paste, glassy carbon, or semiconductor SnO_2. An Ag/AgCl or a saturated calomel electrode (SCE) is used as the reference electrode (RE). The potential scan or sweep is carried out between two potential values of interest (e.g., from about 1.2 to $-0.8V$ vs. SCE). The scan rates can be anywhere from $0.1mV$ to $100V$ or more per second but values between $10mV$ to $400mVs^{-1}$ are frequently used. The current response of processes at a metal electrode are indicative of the nature of the redox reaction at the interface. Experimental results derived from measurements of this kind permit the elucidation of mechanism and the thermodynamic parameters of the process (e.g., charge transfer reaction). Frequently a 'duck-shaped' voltammogram is obtained for redox reactions. The underlying physical mechanism responsible for the 'duck-shaped' profile is based on the interplay between the kinetics of the charge transfer process and mass transport of the charge carriers (oxidants and reductants). These basics of CV and its elegance and simplicity are well known to electrochemists. According to our knowledge, this powerful CV technique was applied for the first time to membrane studies in 1984 with interesting results [6].

For s-BLMs, the essential setups are used. Additionally, a new setup of different design is used in order to measure the electrical parameters more accurately [11]. Briefly, an ideal BLM equivalent circuit is represented, as previously, in which a R_m is connected in parallel with a C_m. Since it is known that the current across R_m increases with the scan rate, the total current (I_t) is given by

$$I_t = I_c + I_R = V/R_m + C_m A \qquad (0.8)$$

where A is the area of the BLM, $I_c = C_m dV/dt = C_m A$, and $I_m = V/R_m$. Thus, I_t is a straight line with the slope $= 1/R_m$ and the intercept $= C_m A$. When the direction of scan is suddenly reserved, the polarity of I_c drops down steeply. The voltammetric curve obtained by such a cycle is a parallelogram from which the R_m and C_m can be evaluated by the slope and intercept, respectively. However, the measured voltammetric curves of s-BLMs are not parallelograms. Instead, they are rising curves of certain regions. Since the performance of the instrument has been found to be correct, the difference must be due to the assumed equivalent circuit, which needs some modification. The total impedance of the whole circuit except the R_m, C_s is the distributive capacitor (on the order of tenth of pF) of the circuit. Using this equivalent circuit, the voltammetric curve obtained from the s-BLM experiment may be better evaluated, the details of which will be published elsewhere [11].

RESULTS AND DISCUSSION

A biosensor is an analytical device incorporating biological sensing elements either ultimately connected to or integrated with suitable transducer, enabling the conversion of specific chemical compound concentrations into digital electronic signal [3,12]. Generally, the biological components used in biosensor construction can be divided into two categories: those where the primary sensing event results from catalysis (such as whole microorganisms, tissue slices, organelles and enzymes) and those which depend on an essentially irreversible binding of the target molecule (that is cell receptors, nucleic acids and antibodies) [1,12]. The essential element, however, in making a successful biosensor is to provide a suitable immobilization have been employed: (i) physical adsorption at a solid surface, (ii) entrapment in polymeric gel or within microcapsules, (iii) cross-linking by means of bifunctional reagents often in combination with (i) and (ii), (iv) covalent binding to a reactive insoluble support. These resulted in numerous matrices which have been used. For biocompatibility, a lipid bilayer such as that in the new BLM system is an ideal choice. In more than past ten years planar bilayer lipid membranes (BLMs) have been suggested to hold promise for practical applications [12]. The idea of using BLMs in biosensor technology is based upon the fact that biological membranes are essentially the Nature's sensors and electronic devices operating through selective transport of ions and/or electrons from one side of the membrane to the other. Besides this important fact the detection in biological environments has to be done by a sensing element that is biocompatible and biomembrane-like, as already mentioned. Let us summarize some recent experiments with planar BLMs and s-BLMs in this field in the following section.

BLMs as Electrochemical Biosensors.

Sensory transduction in living cells is thought to involve a change of electrical parameters across the receptor membrane following a specific binding event at the membrane surface. Advances in microelectronics and biotechnology aroused interest in the development of BLM-based electrochemical biosensors. The existence of ubiquitous interfaces and ultrathin bilayer lipid membranes is expected to play an increasingly important role in the development of biomolecular electronic devices. Since its inception, the BLM separating two aqueous phases has been used mainly as a model of biomembranes, in which a lipid bilayer is a universal structural element. It has been demonstrated that, after suitable modification, BLMs could act as electrodes and exhibit nonlinear properties. We found, for example, that the TCNQ-containing BLM in the presence of an electron acceptor on one side and a donor on the other side, the membrane functioned in the manner of coupled redox electrodes [1,6].

Antigen-Antibody Reaction Studies on s-BLMs.

The ion permeability of micro BLMs less than $10\mu m$ in diameter formed on Milipore and Nuclepore filters was seen to exhibit stepwise reductions in electrical resistance in the presence of Forssman antigen, the appropriate anti-serum, and its complement. The results appear to support the 'hydrophobic doughnut' or transmembrane channel hypothesis, which envisions several polypeptide chains anchoring from more than one terminal complement component to interact with one another within the lipid bilayer. Channel formation in these micro BLMs is believed to be due to the indertion of complement proteins. Concentration and temperature studies were carried our to ascertain that the electrical responses were due to the generation of stable channels by complement across the membrane. The diameter of these channels was estimated to be on the order of $1nm$ [13]. In the present work, we report a feasibility study of an antigen-antibody reaction using s-BLMs for biosensors with electrical detection [14]. The antigen (HBs-Ag–Hepatitis B surface antigen) was incorporated into a s/BLM, which then interacted with its corresponding antibody (HBs-Ab–Monoclonal antibody) in the bathing solution. This Ag-Ab interaction resulted in some remarkable changes in the electrical parameters (conductance, potential and capacitance) of s-BLMs. The magnitude of these changes were directly related to the concentrations of the antibody in the bathing solution. The linear response was very good ranging from 1 to $50ng/ml$ of antibody, demonstrating the potential use of such an Ag-Ab interaction via s-BLM as a transducing device [14].

Embedding of Ferrocene on s-BLMs:

An amperemetric Sensor of Ferri-/Ferro- Cyanide Ions. The redox reactions for a solid supported BLM containing vinyl-ferrocene as an electron mediator have been investigated using cyclic voltammetry. The results have shown that (i) ferrocene can be very easily immobilized in the lipid bilayer on the surface of a metallic wire (s-BLM system). This demonstrates that the s-BLM system offers a novel approach to the electrode modification by a simple way of embedding compounds within BLM, and (ii) ferrocene in a bilayer lipid membrane increases about two orders of magnitude of potassium ferri-/ferrocyanide ion sensitivity over that of the platinum electrode. Recently, substitute ferrocenes were incorporated into s-BLMs on Pt support and investigated using cyclic voltammetry [15,20]. In this connection a number of well known electron mediators such as 1,4 naphtho/quinone, ubiquinone; diaminodurene; anthraquinone-2-sulfonic acid (AQS) have been investigated on a Teflon coated platinum wire, the tip of which has been modified by a self-assembled s-BLM. Electrical capacitance of the s-BLM system was measured as a function of the frequency. The findings of this work are discussed in terms of the electron transfer phenomena and the redox reactions [24].

Hydrogen Peroxide-sensitive s-BLMs.

As described previously [8], the insertion of appropriate active molecules (modifiers) into the matrix of the lipid bilayer should be able to impart the functional characteristics of s-BLMs. We chose TCNQ (tetracyanoquinodimethane) and DP-TTF (dipyridyl-tetrathiafulvalene) as modifiers because of their properties as typical electron acceptor and donor molecules, respectively. It was found that DP-TTF could improve not only the stability but also increased the range of s-BLM's sensitivity to hydrogen peroxide. In contrast, TCNQ-containing s-BLMs did not show much response to H_2O_2. This was not entirely unexpected since TCNQ should behave as an electron acceptor [16].

Modified s-BLMs as pH Sensors.

Of all the ions crucial to the functioning of cellular processes is the hydrogen ion (H^+) which plays the leading role in the enzyme catalysis and membrane transport. Thus, it is not surprising that, the measurement of pH is of the utmost importance. Currently, the pH glass electrode is routinely used in chemical and clinical laboratories. However, the large size and fragility of pH glass electrode preclude their use in many situations such as *in vivo* cell studies and in monitoring membrane boundary potentials. For example, the hydrolysis of membrane lipids by phospholipid enzymes (lipases A and C) changes the boundary potential of BLM (or cell membrane) as a result of local pH change. Additionally, it has been known for many years that BLMs formed from chloroplast extracts exhibited Nernstian behavior as a function of pH [8]. These observations suggest that s-BLMs can be used as a pH probe in membrane biophysical research and in biomedical fields where the conventional glass electrode presents many difficulties. To test our concept, we incorporated a number of quinonoid compounds (chloranils) into s-BLMs. We have found that, indeed, s-BLMs containing either TCOBQ (tetrachloro-o-benzoquinone) or TCPBQ (tetrachloro-p-benzoquinone) responded to pH changes with a nearly theoretical slope $(55+3mV)$ [17]. This new pH-sensitive s-BLM offers prospects for ligand-selective probe development using microelectronic technologies. Related to these experiments is alkali cation sensitivity of crown-ether containing s-BLMs. For example, s-BLMs can be formed from a solution of squalene saturated with cholesterol and a crown ether compound (such as the mesomorphic derivatives of 15-crown-5 and 18-crown-6 compounds) [24]. This mixture not only increased the solubility of crown ether compounds but improved also the stability of the s-BLM formed. Experimental results showed that s-BLMs modified with crown ethers have excellent specificity and fastest response to $[K^{+}]$ in the aqueous solution.

Modified s-BLMs as Ion Sensors.

S-BLMs containing six different kinds of synthesized crown ethers were investigated using cyclic voltammetry. In particular, s-BLMs formed from a liquid crystalline aza-18-crown-6 ether and cholesterol-saturated n-heptane solution were found to be sensitive to K^{+} in the concentration range of 10^{-4} to $10^{-1}M$ with theoretical Nernstian slope [18]. The specificity for three alkali metal cations and NH_4^{+} of five different kinds of bis-crown ethers in BLMs were investigated. The order of specificity for most of these bis-crown ethers was found to follow hydrated radii of cations, i.e., $NH_4^{+} > K^{+} > Na^{+} > Li^{+}$. The results obtained with these s-BLMs compare favorably with conventional BLMs containing similar compounds such as valinomycin [18].

Modified s-BLMs as Molecular Sensors.

Many authors have reported sensors for the detection of glucose using glucose oxidase. Earlier, we have reported immobilization of glucose oxidase on a polypyrrole-lecithin BLM with good results [19]. Interestingly, using s-BLMs containing redox compounds and electron mediators but without the enzyme, glucose was detected in buffered solution. The results are very preliminary and further experiments are in progress. If highly conjugated compound such as TNCQ is incorporated in the s-BLM forming solution, the resulting s-BLM was able to detect the presence of ascorbic acid, which is consistent with the findings obtained with conventional BLMs.

S-BLMs on Interdigitated Electrodes by Microelectronic Techniques.

The results of our recent research have confirmed a broad spectrum of BLM applications [3,12,20]. All of these possibilities are based upon the fact that a lipid bilayer formation overcomes two basic obstacles in the way of the practical utilization of the BLM structure, namely: (i) its stability and (ii) its compatibility with a standard microelectronic technology. As has been repeatedly demonstrated by us and others, the solid supported BLM system (s-BLM) not only possesses the advantages of a conventional BLM structure but additionally gains the new important properties such as (a) a long-term stability, (b) an anisotropic, highly ordered, yet very dynamic liquid-like structure, (c) two asymmetric interfaces, and (d) this type of probe is predestined for microelectronic fabrication. On this last mentioned property, we extended the experiment described above to the interdigitated structures (IDS). IDS are finger-like electrodes made by microelectronic technologies and used in microchip applications [21]. By forming s-BLMs on IDS made on platinum with a window of $0.5mm \times 0.5mm$, we have obtained the following interesting results. First, when an IDS coated with a BLM formed from asolectin, it responded to pH changes with $15 \pm 2mV/$decade slope. The conductance of s-BLMs on IDS was about 50 times higher than the usual s-BLMs. Second, when an IDS coated BLM formed from asolectin plus TCOBQ (or TCPBQ), the pH response was linear with a $50 \pm 1mV$ slope. This very interesting finding suggests that (i) the lipid bilayer, the fundamental structure of all biomembranes, can be attached to an IDS with responses not unlike those found in s-BLM, (ii) this type of structure (i.e., s-BLM on interdigital electrodes) can be used to investigate ligand-receptor contact interactions, and (iii) s-BLMs on an IDS can be manufactured using microelectronic technologies which already exist without the explicit need of special modification. In this connection it should be mentioned that the experiment on IDS-chip modified with a BLM is based on a common basic aspiration. That is to self-assemble a lipid bilayer containing membrane receptors so that a host of physiological activities, such as ion/molecular recognition can be investigated. With IDS-chip modified with BLMs, we now have at last a most unique system for extensive experimentation which will be only limited by our imagination. Thus, insight gained from these studies will guide the preparation of functional BLMs on IDS support [21]. Our aim is to take advantage of microelectronic techniques and apply them to basic and practical research.

CONCLUDING REMARKS

Finally, it should be reiterated that the s-BLM research is highly interdisciplinary. Emphasis has been and will be placed on fundamental research. Our past work has been benefited by cross fertilization of ideas among various branches of sciences. It seems likely that the devices based on smart materials may be constructed in the form of a hybrid structure, for example, utilizing both inorganic semiconducting nanoparticles and synthetic lipid bilayers. The potential use of the s-BLM system for the development of a new class of organic diodes, switches, biosensors, electrochemical photocells, and biofuel cells is anticipated. We consider our approach to be a unique way to study the characteristic of a molecular junction, free from the usual bulk phase effects. Our approach has been based on a melange of ideas gathered from the fields of membrane biophysics, bioelectrochemistry, photobiology, solid-state physics, and materials science [4,12,21].

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SECTION 4: EVENTS

INTERNATIONAL CONFERENCE ON MOLECULAR ELECTRONICS AND BiOCOMPUTING

September 25 - 30, 1994, Goa, India
with the eyes of the organizer
Ratna S. Phadke

International Conference on Molecular Electronics and Biocomputing was held during September 25-30, 1994 in Goa, India under the Chairmanship of Prof. G. Govil, Tata Institute of Fundamental Research, Bombay. This was the 5th in the series of conferences held under the auspices of the International Society for Molecular Electronics and Biocomputing (ISMEBC) and was first time in Asia. It was attended by about 100 participants from Australia, China P.R., Czech Republic, France, Germany, Hungary, Italy, Japan, The Netherlands, Russia, Slovakia, Switzerland, U.K., Ukraine, U.S.A. apart from India. Not only the participants were from near and far, but they belonged to different age groups—from young students, beginners to retired but active eminent scientists. The theme of this series of conferences is of interdisciplinary, multidisciplinary nature. Goa Conference brought together both theorists and experimentalists. It provided common platform to physicists, chemists, biologists, engineers as well as physicians.

Scientific program consisted of Invited Talks, Oral and Poster presentations and Panel Discussions. Moreover, as all participants were housed under a single roof, there were ample opportunities for detailed discussions outside lecture hours. The Conference started with an informal "get-together" which was followed by Prof. P.N. Tandon's Inaugural Talk in which he clearly put forward what medical sciences expect from young fascinating branch of science—Molecular Electronics. Prof. H. Kuhn gave exhaustive review of molecular engineering and supramolecular device—construction, Prof. A. Barraud talked about details, problems and solutions for fabrication of organized molecular assemblies with special emphasis on Langmuir-Blodgett techniques. There were several presentations about LB and self-assembly technique based papers and AFM, STM usage.

There was a special Session on conducting polymers. Papers on Fabrication of molecular memories based on bacteriorhodopsin invited stimulating discussions. A variety of biosensors were described. Noteworthy were views of engineers Prof. D.D. Rossi and Dr. P.R. Apte regarding optimization of sensor characteristics.

In all there were about 50 talks and 30 poster presentations. Poster Sessions were preceded by a short oral briefing on highlights of the work. This helped in converging to a particular poster, a group of scientists working in that and closely related topics, ready with pertinent questions for discussion.

During Panel Discussions which was chaired by Prof. Govil, an account of today's status and future projections of different aspects of Molecular Electronics was taken. Panel, together with the audience concluded that although molecularly assembled computer mimicking human brain-like functions can not be fabricated in foreseeable future, but devices like biosensors, memories, etc. will soon be popular. Moreover, as a spin-off of these endeavours a lot of good basic science will be done.

This conference, held in the beautiful surroundings of Goa beach, was a great success. The desirable characteristics was that both experienced seniors and enthusiastic juniors had equal opportunities for presentation of their work. It is envisaged that the scientific deliberations have sown seeds of novel ideas and collaborative programs which will be presented in the next conference to be held in Japan in 1995.

An informal meeting of ISMEBC, under Chairmanship of Prof. P. Rajczy, was held to understand views and problems of members and perspective members of the Society. There was a general feeling that these days the Society is too passive for satisfactory progress.

A meeting of Indian participants was held with a view to prepare plans for follow up actions. It was felt that National level meetings should be held annually to facilitate exchange of ideas and promotion of collaborative research.

Thanks to International (ISF, IUPAB, NIMA Technology, U.K., TWAS) and National (DST, TIFR) funding agencies, Conference could provide support in one forum or the other (registration waiver, local hospitality, travel grant) to about 80% of the participants. This was particularly useful in maintaining high standards of science content of the conference because good science and availability of finances to a scientist do not always go together.

Ratna S. Phadke
Tata Institute of Fundamental Research
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INTERNATIONAL CONFERENCE ON MOLECULAR ELECTRONICS AND BIOCOMPUTING: ICMEBC'94 in Goa, India

with the eyes of a guest
Michael Schmelzer

The fifth meeting in the series of conferences initiated by the International Society of Molecular Electronics and Biocomputing was held from 25.-30. September 1994. Almost 100 participants, including leading researchers from 17 different countries, attended the symposium which was organized by Prof. Girjesh Govil and Dr. Ratna S. Phadke, both from the Tata Institute of Fundamental Research, Bombay.

47 talks were presented in 13 sessions and two poster sessions completed the scientific part of the conference. The topics were spread over the entire field of Molecular Electronics and Biocomputing. The following is a (probably subjective) selection of some of the most interesting topics.

Prof. Hans Kuhn (Switzerland) gave a talk on present-day attempts in molecular engineering. Supramolecular architectures was the keyword of a presentation given by Prof. André Barraud (Gif-sur-Yvette). Self- Organization and the Langmuir-Blodgett technique were also important topics in several talks reporting on the realization of Molecular Electronic Device concepts like the Molecular Rectifier. Another highlight was the talk on Nanoscale Machining by Dr. Bruce Paul Gaber (Washington). He reported on the research concerning the use of AFM as a molecular machine. The design and synthesis aspects of novel materials with respect to NLO, ferro- and pyroelectricity or applications e.g. in sensor devices were foci in a series of talks. Prototypes for Molecular Wires as presented in the talk of Prof. Neol S. Hush (Sydney), research on (conducting) polymers by Dr. Anasuya Raghunathan (Madras), protein engineering as a tool for tailoring biomolecular properties by Prof. Tony Cass (London) are further contributions which indicate recent research within the experimental section of the field covered in this conference. New theoretical concepts were introduced in a talk entitled Molecular Electronics and Quantum Computation presented by Prof. Günter Mahler (Stuttgart). Another interesting lecture was given by Prof. Stanislav Nešpůrek (Prague). Electron transfer, ion switching and charge carriers in s-conjugated polymers were the topics in his presentation. Dr. Toru Watsuji (Tokyo) gave a contribution on the state of the art research carried out in Japan's Future Electron Device project.

This brief overview already indicates the variety of topics covered. This is probably caused by the title Molecular Electronics and Biocomputing, which brings together scientists of such different fields like physics, chemistry, material science, biology and many more. A unique mixture of researchers is a prerequisite for stimulating discussions. Last but not least, evening events, the beach resort hotel, and a familiar atmosphere were the basis for this Conference with outstanding character.

Michael Schmelzer
Strasbourg-Stuttgart

INTERNATIONAL SYMPOSIA ON BIOMOLECULAR AND MOLECULAR ELECTRONIC DEVICES (5TH) AND MOLECULAR ELECTRONICS AND BIOCOMPUTING (6TH)

Okinawa, Japan

This common meeting of FED and ISMEBC, Symposia BMED'95 & MEBC'95, was held in the Okinawa Zanpamisaki Royal Hotel, Okinawa, Japan, November 28-30, 1995. It followed the earlier BMED Symposia in Tokyo (1985), Fuji-Yoshida (1988), Kobe (1990) and Miyazaki (1992) and MEBC Symposia in Budapest (1987), Moscow (1989), New York City (1991), Gaithersburg (1993) and Goa (1994). It was organized by FED and ISMEBC, sponsored by FED, supported by the Ministry of International Trade and Industry and co- sponsored by 2 international and 10 Japanese professional societies, as well as by 1 international and 1 Japanese institutes.

Two main dominating branches of our multi- and interdisciplinary field were reflected in the program as it was organized by the two leaders of these branches, Prof. Masuo Aizawa, Chairman of the Program Committee and Gen Matsumoto, chairing the Organizing Committee. Molecular assembly, supramolecular materials for bioelectronic devices and systems (A) represented one side of the coin, including about thirty contributions.

Brainware (brain/neural functional information processing and devices), learning and memory (B) showed its other side by about forty presented works, leaving space for roughly thirty works in different other topics representing concurrent researches in fields such as physiology, biochemistry, synthetic chemistry, material engineering, system science, and electronics.

Géza Biczó, Budapest

ERPOS-7
Electrical and Related Properties of Organic Solids

18-22 June 1996

Polanica Zdroj, Poland

Electrical properties:
— charge transport
— photoconductivity and electroluminescence
— organic conductors, semiconductors and superconductors
— functional polymeric systems

Spectroscopy:
— novel spectroscopic techniques (single molecule spectroscopy, spectroscopy of molecules on surfaces and in isolating matrices)
— transient spectroscopy of molecular structures

Nonlinear optics:
— optical nonlinearity
— novel nonlinear optical organic materials
— photorefractive materials
— electro-optic materials and devices
— application of nonlinear optics and laser spectroscopy

Photoinduced transformations:
— photoinduced structural changes
— molecular photochromism
— optical switching and storage devices

Molecular thin films:
— Langmuir-Blodgett films: materials/applications
— organic crystalline nanostructures and superlattices
— thin film sensors

Theoretical methods:
— computer modeling
— simulation methods

International Symposium
OPTICAL INFORMATION SCIENCE AND TECHNOLOGY (OIST'97)

26-30 August,1997

Moscow, Russian Academy of Science

The goal of the Symposium was to discuss new information technologies based on optical memory and neural networks. The Symposium covered different areas of this problem, including architectures and algorithms, implementations and applications of optical neural systems capable of selforganizing and learning. The Symposium was a further development in the series of "Optical Memory and Neural Networks" international conferences held in Zvenigorod (April, 1991) and Moscow (August, 1994).

Symposium Topics
— Fundamentals of Optical Memory and Neural Networks
— Optical Neural Computing and Data Processing
— Optical Bioelectronics and Biocomputing
— Optical Recording Mechanisms and Materials
— Photosensitive Biostructures
— Dynamic Holography and Spectral Hole Burning
— 3D Memory and Interconnects
— Holographic and Diffractive Optics
— Optical and Optoelectronic Components
— New Information Technologies, Systems and Applications

Conference 1: Optical Memory and Neural Networks
— Fundamentals of optical memory
— Holographic and neural memories
— 3D and space-temporal memories
— Photosensitive biostructures and dynamic interconnects
— Architectures, algorithms and implementations of optical neural nets
— New information technologies based on associative learning
— Speech and pattern recognition
— Combinatorial optimization and control systems
— Optical and optoelectronic arrays for parallel and associative processing
— Systems and applications

Conference 3: Recording Mechanisms and Media
— Photochemical reactions and photophysical transformations in organic and inorganic media
— Nonlinear phenomena for optical recording
— Photochromogenic and photochromic materials
— Photoanisotropic media
— Photothermoplastic and photoluminescence media
— Silver halide materials
— Magneto-optical materials

Conference 2: Optical Bioelectronics and Biocomputing
— Biocomputing mechanisms and mathematical modeling
— Optical methods for controlling biomolecular processes
— Light-sensitive biomolecules and media
— Implementations and devices
— Applications

Conference 4: Computer Optics and Holographic Optical Elements
— Theory and modeling
— Computation methods
— Fabrication techniques
— Microoptics technology
— Holographic optical elements
— Lenslet arrays
— Novel optical systems

K.V.Chibisov Memorial Workshop on "Physico-Chemical Processes in Silver Halide Systems"
— Mechanism of latent image formation
— Spectral and chemical sensitization
— Emulsion synthesis
— Development and processing

Workshop on "Coherent Effects in Information Optics"
— Specle pattern interferometry
— Imaging using the coherence function
— Data processing using partially coherent light

ECME'97

4th European Conference on Molecular Electronics

7-10th September 1997

St. John's College, Cambridge

Invited and Contributed Talks

M. Fujihira (Tokyo Insitute of Technology - Tokyo) Molecular photodiodes - Their structures and functions *(invited)*

R.H. Berg (Risø National Laboratory - Roskilde - Denmark) Optical data storage using peptides *(invited)*

I. Willner (The Hebrew University of Jerusalem - Jerusalem) Molecular Optoelectronic and Optobioelectronic Systems *(invited)*

S.H.M. Persson (Chalmers University of Technology, Gothenburg) Single-electron tunnelling devices made by self-assembly of colloidal gold clusters between two electrodes and observation of 0.2V Coulomb blockade

H. Anderson (Dyson Perrins Laboratory, University of Oxford) Conjugated rotaxanes- Insulated dyes and molecular wires

D. Schlettwein (Dept. 2 - Chemistry, University of Bremen) Influence of molecular structure on molecular interactions in substituted phtalocyanine thin films

J.P. Rabe (Humboldt University of Berlin) Self-Assembly and interfacing of macromolecular nanostructures *(invited)*

H. Port (3rd Physical Institute, University of Stuttgart) Near-field molecule-substrate interaction. Perylene dyes on metals and semiconductors

L.C. Venema (Applied Physics and DIMES, Delft University of Technology) Low temperature STM imaging and spectroscopy on individual single-wall carbon nanotubes

C. Taliani (Institute of Molecular Spectroscopy - Bologna) Electronic Structure and Morphology of Ordered Thin Film Architectures *(invited)*

S. Carter (Physics Dept., University of California, Santa Cruz) Enhanced luminance in polymer-nanoparticle composite light emitting devices

K. Murata (Electrotechnical Laboratory, Tsukuba, Japan) Polarization dependence of light-induced ESR for stretch-oriented poly(p-phenylene vinylene) (PPV) films

Y. Shimoi (Electrotechnical Laboratory, Tsukuba, Japan) Theory of Electroabsorption of phenylene based conjugated polymers

M. Berggren (Bell Laboratories - Lucent Technologies - Murray Hill) Materials and resonators for low threshold organic lasers *(invited)*

E. Stathatos (University of Patras) Monochromatic light emission from laser dyes in corporated in thin surfactant films

U. Lemmer (Ludwig-Maximilians-University, Munich) Exciton dissociation and cooperative emission in a ladder-type conjugated polymer

H. Bässler (Dept. of Physical Chemistry, University of Marburg) Transport and recombination of charge carriers in organic LEDs *(invited)*

M. Grell (Dept. of Physics, University of Sheffield) A liquid crystalline main chain conjugated polymer for polarized electroluminescence applications

M. Van der Auweraer (Catholic University of Leuven) Hole injection into molecular dispersions of hole transport materials

W. Brütting (Experimental Physics II, University of Bayreuth) Doping and trap states in PPV Light Emitting Devices

A.P. Alivisatos (University of California - Berkeley) Electrical Characteristics of Semiconductor Nanocrystals *(invited)*

P. Spearman (Laboratory of Molecular Materials, CNRS, Thiais) Photovoltaic devices based on conjugated polymer/CdS composites

G. A. Pagani (University of Milan) Heterocyclic push-pull molecules for light interacting and advanced NLO materials

E.W. Meijer (Technical University of Eindhoven - Eindhoven) Design, synthesis and electronic properties of new macromolecular architectures *(invited)*

R.A.J. Janssen (Organic Chemistry, Eindhoven University of Technology) High-spin cation radicals of aniline oligomers

M. Andersson (Chalmers University of Technology, Gothenburg) Solar cells from poly(thiophenes)/C_{60} blends

M. Burghard (Max-Planck-Institute for Solid-State Research, Stuttgart) Template-directed assembly of ultrasmall metal clusters and π-conjugated molecules into one-dimensional arrays

C. Lapersonne (University of Paris VII and Paris VI) Isolated Polydiacetylene chains as an experimental model system for conjugated polymers: nature and relaxation of elementary excitations *(invited)*

T. Bjornholm (Chemistry Dept., University of Copenhagen) Self-assembly of π-stacked conjugated polymers at air/water interfaces. Structure and properties of Langmuir Blodgett films of amphiphilic regioregular poly(3-alkylthiophene)

M. Pfeiffer (Applied Photophysics, Technical University of Dresden) Controlled doping of phtalocyanine layers by cosublimation with acceptor molecules

A. Dodabalapur (Bell Laboratories - Lucent Technologies - Murray Hill) Organic Transistors: Materials Physics and Charge Transport Phenomena *(invited)*

C. Drury (Philips Research, Eindhoven) Integrated logic circuits made using all polymer transistors

A. Ioannidis (Xerox Corporation, Webster) Electrical properties of Au/polymer interface

R.J.O.M. Hoofman (Radiation Chemistry, Delft University of Technology) Highly mobile electrons and holes on isolated MEH-PPV chains

J.-L. Brédas (University of Mons-Hainault) Electroluminescent conjugated polymers: analysis of the absorption and emission characteristics of isolated and interacting conjugated chains *(invited)*

R. Bozio (Physical Chemistry Dept., University of Padua) Electron-vibration coupling effects in the special pairs of photosynthetic reaction centers

M. Utinans (Organic Chemistry Dept., Riga Technical University) Quantum chemical calculations, synthesis and properties of novel organic molecules with photoinduced intramolecular electron transfer and giant change of electric dipole moment in excited state

S. Alvarado (IBM Research, Zurich) STM-excited luminescence on organic materials *(invited)*

Th. Kugler (Physics Dept., IFM, Linköping University) Electronic and Chemical Structure of Conjugated Polymer Surfaces and Interfaces: Applications in polymer-based light emitting devices

K. Sugiyama (Chemistry Dept., Nagoya University) UV photoemission study of model interfaces for organic EL devices

SECTION 5: NEWS OF THE SOCIETY

Draft of Minutes of the Informal Meeting of the GB

at ICMEBC
29 Sept 1994
Goa, INDIA

Members present: BREHMER, DE ROSSI, METZGER, NEŠPŮREK, PHADKE, RAJCZY

Invited people: BARRAUD, BICZO, CASS, HUSH, WATSUJI

Items discussed:

Elections: There should be an election for the President-Elect for the years 1994 and 1995, also 4-4 members to the GB for both periods 1994-96 and 1995-97.

Proposal: President should be elected for 2 years in the future (DE ROSSI). This would need modification of the Constitution.

Names mentioned: for President: DE ROSSI, KAHN; to GB: TRIPATHY, CASS, BARRAUD.

Symposium: The next official Symposium of MEBC is to be organized by President AIZAWA in Japan, 1995.

Newsletter: NSWC has been supporting the Newsletters ##5,6,7 of MEBC during 3 years. Now the support has been stopped. There is a need to publish the next issue (Newsletter #8) urgently, in order to keep membership informed, and to distribute voting ballots.

Frequency of the Newsletter should not be interior 4/year (NEŠPŮREK). At the same time, BICZO should continue negotiations with publishers.

Mutual advantage could be achieved if 'Newsletter of MEBC' and eventually 'MEBC Letters' would be attached to an already existing (cheap) journal (Nanobiology, Synmetals, Thin Solid Films, ...) (BARRAUD, PHADKE, ...). We could also approach ACS (METZGER).

ISMEBC could become a centre of informations if it would take the role of regrouping informations and reviewing or abstracting papers that appear in rare or exotic journals. (BARRAUD)

Minutes subject to corrections. Further contributions are kindly welcome from the absent members of GB.

Péter Rajczy
Secretary, ISMEBC

Bombay, 5 October, 1994.

1995 MEMBERSHIP BALLOTING

Secretary Péter Rajczy has reported on the results of the recent election.

Official election has been made for ISMEBC officers between April and June 1995. Since there was no election held in 1994—due to technical reasons—voting should be made for the President (1995), the President-Elect (President in 1996), 4 members of the Governing Board (1994-1996) and 4 members of the Governing Board (1995-1997).

ISMEBC 1995 ELECTION BALLOT sheet has been circulated among the membership in April.

In result, the following persons have been elected into the elective offices of ISMEBC:

ELECTED FOR PRESIDENT 1995

DANILO DE ROSSI (Pisa, Italy)

ELECTED FOR PRESIDENT-ELECT (PRESIDENT IN 1996)

MICHAEL C. PETTY (Durham, UK)

ELECTED FOR 8 NEW MEMBERS OF GOVERNING BOARD

1994-1996

Géza Biczó (Budapest, HUNGARY)
Isabelle Ledoux (Bagneux, FRANCE)
Robert. W. Munn (Manchester, U.K.)
Toru Watsuji (Tokyo, JAPAN)

1995-1997

Ratna S. Phadke (Bombay, INDIA)
Brian Pierce (Los Angeles, USA)
Michael Schmelzer (Stuttgart, GERMANY)
Klaus-Peter J. Zauner (Detroit, USA)

Detailed ballot sheets and detailed results may be obtained from the Secretary.

Ann Tate Completes Term as First MEBC Treasurer

Ann Tate, who was instrumental in the founding meeting at Balatonszéplak, has served since 1991 as the first treasurer of ISMEBC. Ann is giving up the treasurer post at this time to pursue advanced university studies. Some of Ann's achievements during her term include raising the newsletter to a new level, securing support for the initial activities of the Society, contributing to the success of the 1993 Gaithersburg meeting, and helping to organize the points of contact system. At the same time she has developed an active research program on molecular computing, focusing in particular on b-r films. On behalf of the Society we want to express our sincere appreciation to Ann for a difficult initial organizing job. We wish her the best of success in her coming studies, and thank her in advance for her continuing and future contributions to the Society.

Michael Conrad (1993 President)
Géza Biczó (Founding President)

MEBC Electronic Communications (MEC)

There is a new service for the public of MEBC in an experimental stage which is using the Internet's possibilities to offer easier information exchange in the topics of Molecular Electronics and BioComputing. It has the following forms

(I) MEBC List and File Server
(II) ISMEBC WWW server "http://mebc.elte.hu/mebc/"
(III) MEBC ftp site "ftp.elte.hu:/pub/mebc"
(IV) MEBC gopher server "gopher.elte.hu"

which are partially overlapping and interacting in order to make choice possible - depending on the user's resources. MEC cannot, of course exist without receiving inputs from its users.

Short description of MEC resources:

(I) MEBC List and File Server

- a Mailing List of ISMEBC has been started for discussion/informing people. Becoming a subscriber of this list can be done simply by writing to the address: mebc-request@ludens.elte.hu
SUBSCRIBE MEBC *your name*

Your letters written to mebc-sender@ludens.elte.hu will be sent out to all subscribers. You are welcome to use it for announcements of conferences and other things of public interest.

- a File Server to be addressed as mebc-doc@ludens.elte.hu containing packages of archived informations, mainly coming from the listserver. They are sent automatically upon the request
SEND package (where package can be DOC, JOBS, MEETINGS, REVIEWS etc)
LIST * (to ask about the contents of available packages)
HELP (to get information about the use of archive)

To appeal (and not to loose later) the interest of its users, the listserver needs to get fresh and essential informations as inputs.

(II) ISMEBC WWW HOME PAGE

As part of the MEC, the ISMEBC now has a page on the WorldWideWeb (www), a fast growing information network initiated by CERN (the European Laboratory for Particle Physics).

The www provides access to text, image and sound, that is stored distributed on computer systems connected to the internet. A typical www page combines text and graphical illustrations with links to other www pages that can be located anywhere within the network. A locally-running browser program (usually available for free) is used as a user friendly interface.

Thousands of research groups and individuals active in all branches of science already have www pages on the network. Typically such pages provide information to contact the group or the person, a short summary of the research activities and often a bibliography.

There are two ways to retrieve a page: If the address of the page is known
— e.g., for the ISMEBC page this address is:

http://mebc.elte.hu/mebc/

— it can directly be entered into a browser program. Second, a www page can build a connection (called a hypertext link) to any other www page. Such a connection allows the user to retrieve connected pages by pointing and clicking with the mouse.

We intend to provide links from the ISMEBC page to pages of all research groups that work in the field of MEBC. We will register the ISMEBC page with the www search engines so that a search for MEBC keywords can be followed by pointing and clicking to any research group. If your research group or department has a www page, please look at the ISMEBC page where you will find information on how to enter the page of your group into the list of MEBC research groups.

As another service of the MEC, we intend to maintain a list of recent publications in the field of MEBC. It appears, that in such an interdisciplinary field as MEBC, a common bibliography would be helpful. This bibliography will be made available through the MEC ftp site and also accessible by gopher and www. Please send files with entries by e-mail to kjz@cs.wayne.edu (or kjz@jupiter.cs.wayne.edu), preferably in BibTeX format. As long as the load will not be to high, any file format will be accepted and an attempt will be made to convert it.

(III) MEBC anonymous ftp site

"ftp.elte.hu:/pub/mebc" is a mirror site of mebc-doc@ludens.elte.hu for interactive use.

(IV) MEBC gopher server

"gopher.elte.hu" is a mirror site of ftp.elte.hu for users who prefer gopher to WWW.

Péter Rajczy

Informal Meeting of the Governing Board at MEBC'95

An informal meeting of the Governing Board (GB) was held during MEBC'95 November 29 under the chairmanship of Immediate Past President M. Aizawa. From the GB were present: M. Aizawa, G. Biczó, R. Phadke, T. Watsuji and K.-P. Zauner. The present GB members invited G. Matsumoto and N. Rambidi from the nomination committee as well as T. Cass and M. Conrad to attend the meeting.

After a brief discussion of the results of the past election, the issue of the open treasurer position was of concern. Currently the Secretary Péter Rajczy is interim treasurer and the funds of the Society have been transferred to Hungary. It was agreed upon that the important position should be filled soon and with someone in a country that allows for easy monetary transactions. Further it was felt that a new nomination committee, possibly with fewer members should be assembled. This has to be done soon, since a the nomination of four new GB members is necessary.

An issue that came up in the discussion was the possible extension of the presidency from the current one-year-period to two years. This would require a change of the Society's constitution. M. Conrad commented that it is desirable to have the secretary and the treasurer in their positions as long as they are willing to serve in these functions.

The upcoming ISMEBC meeting was considered at length and possible future meeting sites were discussed. Madam Yu Wei has offered to organize a meeting in China. The decision to hold such a meeting in China was agreed to by the GB at the Gaithersburg meeting in 1993. Since the last two meetings were held in Asia the possibility of a meeting site in Europe was also considered (again in accordance with decisions made by the GB in 1993).

Cooperation of the ISMEBC with a SPIE meeting to be held in Moscow 1997 was proposed by N. Rambidi. The SPIE meeting will include a symposium on 'Optical Bioelectronics and BioComputing'.

M. Aizawa inquired about the situation of the newsletter no. 8. G. Biczó had a draft copy of the nearly finalized newsletter, assembled by Péter Rajczy and himself, at hand and mentioned that the production was delayed due to several absent contributions. There was a strong consensus, that the newsletter is of great importance for communication with the members. A shorter, but more frequently appearing newsletter may better serve this purpose.

A number of other topics that entered the discussion included: tracking the membership, communication with the POCs and members, proxies from absent board members, collecting dues and the general infrastructure of the Society. G. Biczó and T. Cass pointed out that M.C. Petty expressed his intention to address these problems during his presidency.

Respectfully submitted,
Klaus-Peter Zauner

SECTION 6: COMING EVENTS

MEBC-7
THE 7th INTERNATIONAL CONFERENCE ON MOLECULAR ELECTRONICS AND BIOCOMPUTING

November 10-12, 1997

Southeast University, Nanjing, P.R.China

ORGANIZED BY

National Laboratory of Molecular and Biomolecular Electronics Southeast University

International Society of Molecular Electronics and Biocomputing

SPONSORING ORGANIZATION

National Natural Science Foundation of China

State Education Commission of China

K.C. Wong Education Foundation, Hong Kong

Chairperson:

Yu Wei, Nanjing, China

Secretary General:

Z.H. Lu Nanjing, China

Invited and Oral Talks:

Molecular Electronics: An Important Part of Information Science Yu Wei (Vice minister, the State Education Commission of China)

Conformation-Driven Computing: A Comparison of Designs Based on DNA, RNA, and Protein Michael Conrad (Wayne University, USA)

Chemical Sensor Based on Thin Organic Films Michael C. Petty, (University of Durham, UK)

Superconductivity in Molecule-Based Solids Takehiko Ishiguro (Kyoto University ,Japan)

Neural Networks Based on Biomolecular Nonlinear Dynamic Media : State of Art and Some Potentialities Nicholas G. Rambidi (Internal. Res. Inst. of Mag. Sci., Russia)

Supramolecular Architectures for Micro-Sensorics and Molecular Electronics Ludwig Brehmer (University of Potsdam, Germany)

A New Approach for Fabrication of A Self-Organizing Films of Heterostructured Polymer/Cu2S Nanoparticles Xi Zhang (Jilin University,China)

Chiral Metallocene-New Generation of Polymerization Catalysts Ju Zheng Liu (Southeast University , China)

Rectification Characteristic of Cu-TCNQ Organometallic Crystallite Device Ning Gu (Southeast University, China)

Fabrication of Nanoparticulate Mirostructures Using Self-Assembled Methods Jun Fu Liu (Southeast University, China)

Laser Assisted Deposition of Preformed Organizates Ratna S. Phadke (Tata Institute of Fundamental Research, India)

Observation of Molecular Alignment of N-Octadecyl by Scanning Tunneling Microscope Pu Qian (Tohoku National Industrial Research Institute, Japan)

Designing of Protein Based Color Sensitive Retina Frydrych Jussi P. S. Parkkinen (Lappeenranta University of Technology, Finland)

Enzyme Cascades in Biorecognition Judith Rishpon (Tel-Aviv University,Israel)

Influence of Polymerization Conditions on Morphologies of Polypyrrole Chunwei Yuan (Southeast University, China)

Studies of Nanoparticulate Cadmium Sulfide in Amphiphilic Polymaleic Acid Octadecanol Ester Langmuir-Blodgett Films Jian Jin (Jilin University, China)

Some neural network learning schemes for invariance extraction Han Chuan Peng (Southeast University , China)

A Learing and Memory Model in the Speaker Recognition System Jun Yao(Southeast University, China) Poster Oral Presentation

The Role of High - Fidelity separation in DNA Computing David Wood (University of Delaware, USA)

Molecular Assembly and Organized Molecular Films Zu Hong Lu (Southeast University, China)

Molecular Engineering in Bioelectronic Devices Tetsuo Moriya, (Electrotechnical Laboratory,Japan)

Ink-Jet Sterolithography of Poly (3, 4- Ethylenedioxythiophene) Planer and D Structures Danilo Derossi, (Pisa University,Italy)

Molecular Beam Epitaxial Growth of Organic Thin Films on Semiconduction Substances Atsushi Koma (University of Tokyo, Japan)

Molecular orinetation of photosynthetic reaction centers Jun Miyake, (NAIR, AIST/MITI, Japan)

Bacteriorhodopsin - How far to its technical application? Nobert Hampp (Philipps Unversity Marburg,Germany)

Application of Nanometer Particles in The Biomimetic Films Long Jiang (Inst.of Photographic Chemistry, Sinica, China)

Conformation-Driven Computing: The Context-Conformation-Action Loop Simulated Klaus-Peter Zauner (Wayne State University, USA)

Reactivity of Organic Solids and Molecular Electronics Eliana Tapuhi (Tel-Aviv University, Israel)

Structural, Magnetic and Mossbauer studies of Oxalato-Bridged Bimetallic Ferro and Ferrimagnets Peter Rajczy (Eotvos University,Hungary)

Synthesis and Characterization of Functionalised Silicon Phthalocyanines for Fabrication of self-Assembled Monolayers Marya Lieberman (University of NotreDame,USA)

Syntheses and Electrochemical Characterization of Redox Polypeptides as Molecular Electrical Wire Hiroaki Shinohara, (Okayama University,Japan)

Protein Engineering for Self-Assembling Protein Molecular Networks on solid Surface Masuo Aizawa (Tokyo Institute of Tech., Japan)

Photoelectric molecular sensors: molecular origin of differential responsivity Felix T. Hong (Wayne University,USA)

Self Assembly of Aromatic Molecules Over Zeolite (010) Surfaces: An AFM and Semiempirical Study Masaharu Komiyama (Yamanashi University, Japan)

A Jordan One Is Behind the Van Hove Scenario. Towards A Quantum Chemical Theory of High Temperature Superconductivity Geza Biczo (Hungarian Academy of Science, Hungary)

STM Imaging and Manipulation of DNA Molecules Adsorbed on Cu(111) Surface Tomoji Kawai (Osaka University, Japan)

(For more information, please contact the www page of the conference, http://202.119.18.100/, or mail Dr. Haiqian Zhang, zhq@seu.edu.cn)

THE BIOS '98 SYMPOSIUM PHOTONICS WEST '98

24-30 January 1998, San Jose Convention Center
San Jose, California USA

Biomedical Sensing, Imaging and Tracking Technologies III

Conference Chairs:

Robert A. Lieberman, Physical Optics Corp.; Tuan Vo-Dinh, Oak Ridge National Lab.

Program Committee:

Irving J. Bigio, Los Alamos National Lab.; David M. Harris, Bio-Medical Consultants, Yale Univ. School of Medicine, Univ of Illinois School of Dentist; Hong Liu, Univ. of Massachusetts; Fred P. Milanovich, Lawrence Livermore National Lab.; G. Wayne Morrison, Oak Ridge Ctr. for Manufacturing; Halina Podbielska, M.D., Technical Univ. of Wroclaw (Poland); H. Ti Tien, Michigan State Univ.; William R. Wiesmann, M.D.,

Space Biosciences

Conference Secretary: Julia B. Cooper, Oak Ridge National Lab.

The goal of this conference is to provide a multidisciplinary forum for state-of-the-art methods and instrumentation for biomedical sensing, imaging, and tracking technologies.

A forum that integrates interdisciplinary research and development is critically needed for scientists, engineers, manufacturers, and clinical providers to present the most recent advances in instrumentation and methods as well as clinical applications in the important areas of minimally invasive techniques and systems (other than currently developed modalities, i.e., x ray, CSI, MRI, EIT, and magnetic source imaging), pathological spectroscopy, PDT, and optical tomography.

The focus is in the following topics:

Biomedical Sensors

A wide variety of biomedical sensors including fiber optic chemical sensors and biosensors have been developed recently for clinical monitoring of blood pressure, blood chemistry, pH, temperature, and the presence of pathological organisms or biochemical species of clinical importance. Papers are invited in the following and related areas:

— physical/chemical sensors and direct spectroscopy — chemical/blood gas sensing techniques and devices — biosensors (enzyme, antibody, gene probe-based systems) — novel and advanced concepts — component/system design, engineering, and performance — clinical applications

Bioimaging Techniques and Devices

Recent alternative concepts and technologies are emerging in the important area of bioimaging. Many technologies, originally developed for other applications (e.g., defense, energy, aerospace) have found uses in medical applications. Papers are solicited on the following or related topics:

— advanced detector/imaging techniques and systems (CCDs, CIDS, KCDs, selenium detectors) — IR, ultrasound, and acoustic sensing and imaging — advanced endoscopy techniques and devices — smart catheters — laser radar sensing and imaging — RF radar imaging — storage phosphor systems — advanced storage phosphor systems — cardiac mapping — trauma care — telemedicine — virtual reality technologies

Bionavigation and Tracking

From the brain to the sinuses to the abdomen, precision navigation and tracking techniques are critical to position medical instruments precisely within the 3D surgical space. For instance, stereotactic systems are being developed for brain surgery and flexible micronavigation devices engineered for medical laser ablation treatments. Papers are solicited on the following and related topics:

— tracking technology (optical, acoustic, etc.) — stereotactic technology — catheter navigation — anatomical landmark identification — robotics-assisted surgery — virtual reality techniques — novel noninvasive navigation techniques

This conference is just one of 33 topics to be held at the BiOS '98 symposium, which is part of the larger event called Photonics West '98: 24-30 January 1998 San Jose Convention Center San Jose, California USA

For a printed BiOS '98 call for papers or other information:
E-mail: pw98@spie.org
Fax: 360/647-1445
Phone: 360/676-3290

IMPORTANT DEADLINES

Camera-Ready Abstracts due from Authors: 24 November 1997
Manuscripts Due from Authors: 29 December 1997 (post-meeting proceedings)

For more informations contact:
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Call for Papers 11th INTERNATIONAL CONFERENCE ON INDUSTRIAL& ENGINEERING APPLICATIONS OF ARTIFICIAL INTELLIGENCE & EXPERT SYSTEMS

IEA-98-AIE

New Methodologies, Knowledge Modeling and Hybrid Techniques

Hotel Intur Orange, Benicassim, Castellon, Spain

June 1-4, 1998

Sponsored by:
International Society of Applied Intelligence
Universidad Jaume-I de Castellon
Universidad Nacional de Educacion a Distancia (UNED), Madrid

In Cooperation with:
AAAI, ACM/SIGART, ECCAI, AEPIA, CSCSI, IEE, IM& C, INNS/SIG, JSAI and SWT

For more information you can visit our web site:

http://titan.inf.uji.es/IEA98/

The 11th International Conference on Industrial & Engineering Applications of Artificial Intelligence & Expert Systems, will take place in Benicassim, Castellon (Spain), June 1-4, 1998. This annual conference on applied Artificial Intelligence and Knowledge Based Systems (KBS) in industrial and engineering environments was first held in Tennessee and then subsequently in South Carolina, Hawaii, Paderborn (Germany), Edinburgh, Austin (Texas), Melbourne (Australia) and, finally, in Fukuoka (Japan'96) and Atlanta ('97). Now, it visits Spain for the first time.

On this occasion the conference will focus on methodological aspects in the development of KBS's, knowledge modeling and hybrid techniques that integrate the symbolic and connectionist perspectives in industrial applications of AI. Papers will be accepted either for oral presentation or for poster sessions. All papers will be published in full length.

PROCEEDINGS

The Proceedings will be published in time for distribution at the conference as a volume of the Springer Lecture Notes in Artificial Intelligence.

SCOPE

The IEA/AIE-98 Program Committee recognizes the complexity of the real industrial world. To advance the applied perspective of AI we need to examine the characteristics of the scenarios in which generic tasks (such as identification, monitoring, diagnosis, prediction; repair, control, supervision; design and planning) are found to be adequate to the development of KBS's; then, more emphasis is needed on methodology for the phases of development (knowledge modeling, reduction process, development environments and prototype implementation) and techniques (symbolic, connectionist or hybrid). Finally, we need to evaluate the results using "real testbed" and refine again by means of learning. The essential aim of this perspective for the 11th IEA/AIE conference is to reduce the distance between the techniques for modeling and design of KBS's and the engineering procedures normally employed in the analytic and algorithmic perspectives of continuous and discrete systems theory.

INVITED SPEAKERS

The following invited speakers have confirmed their willingness to participate in the conference:

Prof. Michael Brady, Oxford University. Associate Editor of the Artificial Intelligence journal. Prof. Bob J.

Wielinga, University of Amsterdam. Developer of KADS modeling paradigm. Prof. Roberto Moreno, Universidad

de Las Palmas de Gran Canaria, Director of the International Computer Science Research Center. **TOPICS**

1. Methodological Aspects
   1.1 Knowledge modeling
   1.2 KBS development methods and tools
   1.3 KADS related approaches
   1.4 Reverse engineering

2. Formal Tools
   2.1 Analytic and logic models
   2.2 Fuzzy knowledge representation and inference
   2.3 Uncertainty and causal reasoning tools
   2.4 Bayesian networks
   2.5 Qualitative reasoning
   2.6 Neural networks
   2.7 Genetic algorithms & genetic programming
   2.8 Object oriented formulations
   2.9 Hybridization techniques

3. Generic Tasks of Analysis in IEA/AIE
   3.1 Computer vision, intelligent sensors and multisensor perception
   3.2 Speech recognition
   3.3 Natural Language Understanding
   3.4 System identification
   3.5 Monitoring
   3.6 Heuristic and connectionist classification
   3.7 Fault diagnosis
   3.8 Predictive models
   3.9 Design recovery

4. Synthesis Tasks in IEA/AIE
   4.1 CAD/CAM functionalities
   4.2 Spatial, temporal and spatio-temporal planning and scheduling
   4.3 Robotic manipulators
   4.4 Incremental design
   4.5 System configuration

5. Modification Tasks
   5.1 Knowledge-based control systems
   5.2 Intelligent supervision
   5.3 Communication systems (modems-codecs, network management and digital communications)
   5.4 Fault tolerant and self-repair systems
   5.5 Predictive and model-based control systems
   5.6 Visuo-motor coordination
   5.7 Real time in AI applications (architectures, tools and case studies)
   5.8 Perceptual robotics

6. Machine Learning
   6.1 Inductive and deductive strategies
   6.2 Analogy and case-based learning
   6.3 Multistrategy and hybrid formulations
   6.4 Learning in neural nets (supervised and non-supervised)
   6.5 Self organization, synergetics and evolutive optimization

7. Applied AI and KBS's in Specific Domains
   7.1 Development environments in KBS's and neural nets
   7.2 Knowledge editing tools
   7.3 Multimedia
   7.4 Human-computer interaction
   7.5 Decision support systems
   7.6 Tutoring systems
   7.7 Exploratory prototypes
   7.8 Reports on real applications with significant findings

8. Validation & Evaluation Criteria
   8.1 Simulation
   8.2 Validation & Verification

8.3 Reliability, validity, acceptance and legal reasons in different fields of application (aviation, nuclear power plants, alarms, medicine)
8.4 Benchmarks
8.5 Acceptability
8.6 Explanatory capacity

CALL FOR INVITED SESSIONS

The Program Committee is soliciting proposals for invited sessions, particularly in one of the above theme areas. Prospective organizers should first contact the Program Co-Chair A.P. del Pobil at iea98@titan.inf.uji.es, as soon as possible, providing a title for the invited session and including a brief statement of the purpose as well as names of prospective authors if available. Each invited session will consist of four/five papers, if more papers are submitted, then the session can be split into two ones.

The organizer will be responsible for inviting authors, selecting the four papers and submitting four copies of each paper to A.P. del Pobil by November 7, 1997, at the address below. The papers will be reviewed by only one member of the Program Committee (contributed papers are reviewed by at least two members). In case an invited paper is finally not accepted, it will be replaced by a relevant contributed paper. The organizer will be invited to serve as Chair for the invited session at the conference and will be granted a reduced registration fee. Information about current invited sessions can be found at our web site.

IMPORTANT DATES

Submission of papers	November 7, 1997.
Acceptance notification	January 25, 1998.
Camera-ready copy due	February 25, 1998.

For information, contact:

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WWW: http://titan.inf.uji.es/IEA98/