Czech Technical University in Prague
Faculty of Nuclear Sciences and Physical Engineering

České vysoké učení technické
Fakulta jaderná a fyzikálně inženýrská

Ing. Irena Kratochvílová, Ph.D.

Molecular Nanosystems

Molekulární nanosystémy

Summary

Current research in mesoscopic physics focuses on the design and implementation of nanometer scale electronic systems that exhibit new and interesting classical and quantum mechanical effects. The motivation for creating such structures has been two-fold: first, to create nanoscale laboratories to explore physics in a new regime, and second to develop novel devices with significant applications.

Recently, there have been significant advances in the fabrication and demonstration of individual molecular wires and diode switches [1,2].

There also have been advances in techniques for making reliable electrical contact with such electrically conducting molecules. These promising developments in the field of nanostructures suggest that it might be possible to build and to demonstrate somewhat more complex molecular electronic structures that would include more molecular electronic diodes [3,4].

Working with molecular nanosystems we established the formation of metal/SAM/metal junctions inside nanowires through combined electroplating/electroless plating and template replication. Using alkanethiol molecules we tested the nanowires functionality and found that parameters of our molecules in nanowires were close to tabulated molecular parameters. On the molecular wires containing 4-[[2-nitro-4-(phenylethynyl) phenyl] ethynyl] benzenthiol molecules the current-voltage characteristics exhibited at room temperature negative differential resistance with on-off peak-to valley ratio 2.21. Thus novel method how to prepare nanostructure containing organic molecules with negative differential resistance (NDR) property has been worked out. We also modeled the influence of the static electric field and charge variation. The main reason for the peak observed in *I-V* curves is probably associated with the fact that in self assembled monolayer containing NO_2, charge transfer occurs due to reduction from the chemically bonded end involving the level closest to the Fermi energy.

Souhrn

Je zjevné, že se současný výzkum zaměřuje práci se systémy o naorozměrech. Kromě praktické výhody je jistě důvodem i široká škála zajímavých specifických klasických i kvantových efektů. Motivace k práci na této tematice je dvojí: jednak vytvoření vhodných laboratoří pro fyzikální výzkum nové oblast a jednak vytvoření nových prvků s významnými aplikacemi.

V poslední době bylo dosaženo významných úspěchů v přípravě molekulárních vodičů a diodových přepínačů [1,2].

Dále byl učiněn významný pokrok v přípravě molekulárních vzorků se spolehlivými elektrickými kontakty. Tento slibný vývoj na poli nanostruktur dává šanci vytvořit komplexní molekulární elektronické struktury, obsahující více molekulárních diod [3,4].

V přednášce je popsán způsob integrace organických molekul do elektrického obvodu. Vytvořili jsme nanotyčinky obsahující svazky organických molekul za použití kmbinovaného elektrolytického pokovení. V nanotyčinkách obsahujících molekuly alkanthiolu jme testovali funkčnost celých systémů kov-molekula-kov. Důkazem funkčnosti systému byla malá změna elektronové afinity alkanthiolových molekul po procesu integrace v nanotyčinkách. Volt-ampérová charakteristika nanotyčinek, obsahujících molekuly 4-[[2 – nitro - 4-(phenylethynyl) phenyl] ethynyl] benzenthiol vykazovala záporný diferenciální odpor. Poměr maxima k minimu v oblasti píku volt-ampérové charakteristiky byl 2.21. Z teoretického molelu vyplývá, že hlavním důvodem záporného diferenciálního odporu je s největší pravděpodobností přesun náboje redukcí z chemicky na zlato vázaného konce molekuly, z hladin nejbližších Fermiho hladině.

CONTENTS

I. Introduction

This lecture is devoted to my work with nanosystems, especially nanosystems containing organic molecules – molecular electronics [5,6]. Molecular electronics has an ambitious but realistic goal: the use of synthesis, assembly and miniaturization on molecular level to achieve huge densities of devices such as molecular wires, rectifiers, switches, transistors and memories. Remarkable progress has been made in recent years in identifying candidate molecules with interesting electronic properties such as molecular conduction, rectification, negative differential resistance and configurable switching. The broad variety of electronic functions available by synthetic modification of these molecules suggests many ways in which they may be used in hybrid or "post-silicon" applications. Here we present current-voltage (I-V) measurements on rod-shaped nanowires using alkanethiol and 4-[[2-nitro-4-(phenylethynyl) phenyl] ethynyl] benzenthiol (NDR) molecules as the active component. We worked with systems that have a metal top contact, self-assembled monolayer (SAM) active region, and a metal bottom contact. Formation of a metal/SAM/metal junction was established inside nanowires through combined electroplating/electroless plating and template replication

Using alkanethiol molecules we tested the nanowires functionality and found that parameters (important for our devices functionality) of our molecules in nanowires were close to tabulated molecular parameters. So we were able to construct nanorods with different properties simply using different types of molecules [7].

Using SAMs of and alkanethiol self-assembled monolayer (SAM) containing NDR molecules the current-voltage characteristics exhibited at room temperature negative differential resistance with on-off peak-to valley ratio 2.21. Thus novel method how to prepare nanostructure containing organic molecules with NDR property has been worked out [8].

The influence of the static electric field and charge variation were modelled. The interaction with the gold electrode influences the electronic structure of the NDR molecule nevertheless the main reason for the peak observed in I-V curves is associated with the fact that in self assembled monolayer containing NO_2, charge transfer occurs due to reduction from the chemically bonded end involving the level closest to the Fermi energy. This charge resides in a molecular orbital which, being partly occupied, lie close to the Fermi level. When charge is transferred and the molecular orbital closest to the Fermi level is

occupied the main remaining electron transport through the molecule is tunnelling (as demonstrated earlier [9]) so the level of the current drops down very rapidly. The overall picture can be influenced by the applied electric field [10].

II. Molecular Nanosystems

Current research in mesoscopic physics focuses on the design and implementation of nanometer scale electronic systems that exhibit new and interesting classical and quantum mechanical effects. The motivation for creating such structures has been two-fold: first, to create nanoscale laboratories to explore physics in a new regime, and second to develop novel devices with significant applications.

Recently, there have been significant advances in the fabrication and demonstration of individual molecular wires and diode switches [11]. There also have been advances in techniques for making reliable electrical contact with such electrically conducting molecules. These promising developments in the field of nanostructures suggest that it might be possible to build and to demonstrate somewhat more complex molecular electronic structures that would include two or three molecular electronic diodes and that would perform as digital logic circuits.

One possible solution to these problems is to use nanowires as carriers of the electronically active molecules. Metal nanowires can be easily fabricated by several techniques. We and others have studied nanowires made by electrochemical template replication. They can be nanoscopic in diameter but macroscopic in length. Therefore, it should be relatively easy to configure composites of nanowires and conducting molecules (molecular wires or electronically active molecules) in electronic circuits compared to wiring individual molecules. Here we present current-voltage (*I-V*) measurements on rod-shaped nanowires using alkanethiol molecules as the active component. We worked with systems that have a metal top contact, self-assembled monolayer (SAM) active region, and a metal bottom contact.

N-mercaptohexadecanoic acid - $HS(CH_2)_kCOOH$, $k=10$ or 15 (referenced as C_{11} and C_{16}) was used for the molecular measurements reported here. Nanowires were prepared using replication inside the 70-nm diameter pores of polycarbonate track etched membranes [12].

Au was electrochemically deposited about half way through the 6 μm long pores and a SAM was adsorbed on top. The high affinity of Au for thiol group results in oriented SAM terminating in carboxylate group. It is particularly important to prevent the plating of metal through defects in the monolayer, which would

7

connect the two portions of the nanowires. To prevent this electrical shorting, an electroless plating procedure [13, 14] was used. A thin layer of electrolessly deposited Au or electroplated Ag formed a cap on the top of the SAM. The remaining empty portion of the pores was then filled by electroplated Au or Ag, producing a nanowire consisting of a bottom electroplated portion, separated from the top portion by an organic monolayer .

Electric-field assisted assembly was used to assemble nanowires for testing electrical properties of rods containing molecules. Lithographically defined arrays were prepared using a 3-mask process. The bottom level consisted of 50 nm Ti/150 nm Au bus bars, which were isolated from the next level by a 4 μm thick layer of benzocyclobutene or a 2 μm thick SiO_2 layer. The next level was an interdigitated array of alignment fingers with separation distance varying from 2 μm to 6 μm. The third level consisted of contact pads that were vapor deposited on top of the aligned nanowires and could be contacted with measurement probes. A 35 V_{rms} AC field was applied, and a suspension of nanowires in dichloromethane placed on the substrates. The wires align across the fingers in response to the applied field. The substrate was then washed with dichloromethane and the contact pads applied. An SEM picture of an aligned rod between two electrodes is shown in Fig.11. Upper electrodes (alignment pads) cover electrodes made for position the nanowires (busbars). The rod containing alkane molecule is approximately 7 μm long and 70 nm thick see Fig. 1. *I-V* characterization of nanowires containing organic molecules (Figs. 2, 3) was done at room temperture by a two-point probe method using a HP 4155 semiconductor parameter analyzer.

Our main goal was to find out the type of electrical transport in molecules and the parameters of this transport mechanism. We assumed that the tunneling process dominates injection of charge carriers in the absence of localized states, i.e., electrons and holes tunnel from metal to the LUMO or HOMO, respectively, of the molecule. The probability of electrons having enough thermal energy to surmount the potential barrier is relatively low, even at room temperature. In this simplified case the injection current from the metallic electrode can be described using Fowler-Nordheim approximation of the probability that the charge carrier can penetrate   through the potential barrier. Our device can be seen as two metal plates parallel to each other and separated by the SAM layer, so the electric field strength is proportional to the voltage difference between metal electrodes.

$$I(V) \approx \frac{V^2}{d^2} \exp(-\frac{Kd}{V})$$,
(1)

where

$$K = \frac{8\pi\sqrt{2m^*}\varphi^{3/2}}{3qh}. \tag{2}$$

These expressions have been used to determine barrier heights at metal/polymer interfaces. By doing so, it is necessary to assume a value of the effective mass of the charge carriers. Furthermore, the film thickness must be precisely known for the considered contact between both charge injection contacts. A good method of metal-molecule-metal structures characterization, in which the charge transport is controlled via the Fowler-Nordheim tunelling, must avoid to need the value of the molecular film thickness and charge carriers effective mass. We were able to construct the gold-molecule-silver systems. An *I-V* curve of such device includes the tunelling current of electrons injected from metal 1 to molecule and to and form metal 2 to molecule for positive and negative bias respectively. These injection currents presents different behaviour, because they pass through a different matal-molecule interface. To each part of the *I-V* curve the following derivative can be calculated:

$$\alpha_i = \frac{d\ln(IV^{-2})}{dV^{-1}} = -Ad\varphi^{3/2} \tag{3}$$

i=1,2

and

$$A = \frac{8\pi\sqrt{2m^*}}{3qh} \tag{4}$$

V - voltage applied on metal-molecule-metal system ,*q* - elementary charge,*h* - Planck's constant, *m** - effective mass of the charge carrier , *d* - the barrier thickness, *φ* - the metal - molecule interface barrier height.

$$I(V) \approx \frac{V^2}{d^2}\exp(-\frac{Kd}{V}), \tag{5}$$

where

$$K = \frac{8\pi\sqrt{2m^*}\varphi^{3/2}}{3qh}. \tag{6}$$

These expressions have been used to determine barrier heights at metal/polymer interfaces. By doing so, it is necessary to assume a value of the effective mass of

the charge carriers. Furthermore, the film thickness must be precisely known for the considered contact between both charge injection contacts.

A good method of metal-molecule-metal structures characterization, in which the charge transport is controlled via the Fowler-Nordheim tunelling, must avoid to need the value of the molecular film thickness and charge carriers effective mass. We were able to construct the gold-molecule-silver systems. An *I-V* curve of such device includes the tunelling current of electrons injected from metal 1 to molecule and to and form metal 2 to molecule for positive and negative bias respectively. These injection currents presents different behaviour, because they pass through a different matal-molecule interface. To each part of the *I-V* curve the following derivative can be calculated:

$$\alpha_i = \frac{d\ln(IV^{-2})}{dV^{-1}} = -Ad\varphi^{3/2} \tag{7}$$

i=1,2

and

$$A = \frac{8\pi\sqrt{2m^*}}{3qh} \tag{8}$$

V - voltage applied on metal-molecule-metal system ,*q* - elementary charge,*h* - Planck's constant, *m** - effective mass of the charge carrier , *d* - the barrier thickness, φ - the metal - molecule interface barrier height.

The barrier height at the interface is the difference between metal work function Φ and the molecule electron affinity χ for electron injection:

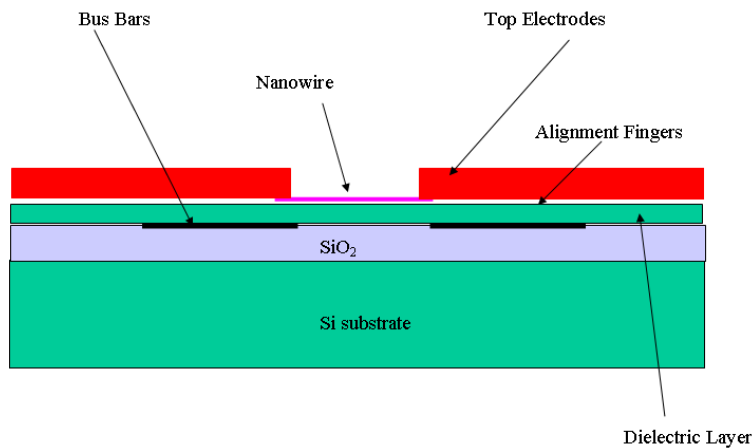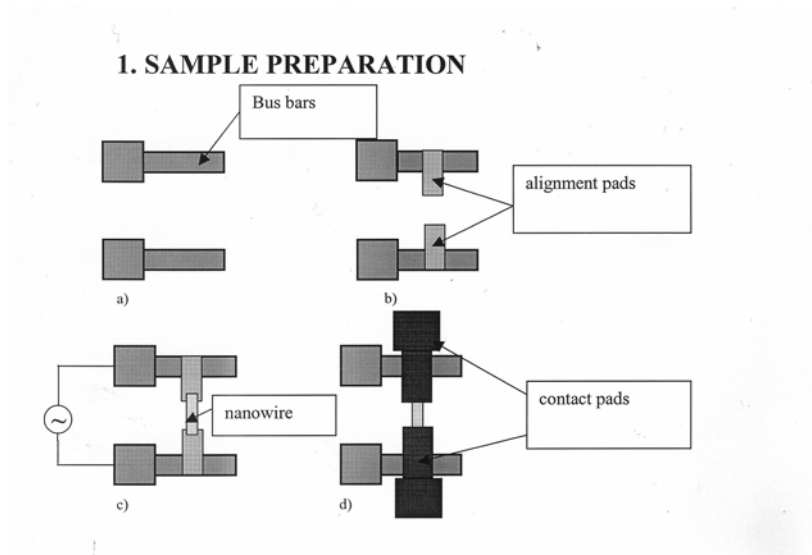$$\varphi_n = |\Phi| - |\chi|. \tag{9}$$

1. SAMPLE PREPARATION

Fig.1: Lithographically defined arrays were prepared using a 3-mask process. Au bus bars, which were isolated from the next level by a 2 μm thick SiO$_2$ layer. The next level was an interdigitated array of alignment fingers with separation distance varying from 2 μm to 6 μm. The third level consisted of contact pads that were vapor deposited on top of the aligned nanowires and could be contacted with measurement probes.

And the barrier height at the interface is difference between molecule ionization potential   μ and the metal work function Φ for hole injection

11

$$\varphi_n = \left| \mu \right| - \left| \Phi \right|.$$

(10)

If we divide α_1 by α_2 we obtain a numerical relation between φ_1 and φ_2 which is independent of the film thickness and charge carrier effective mass, d and of the charge carrier effective mass. Assuming again that the rigid band model is valid, we can write

$$\frac{\alpha_1}{\alpha_2} = \left(\frac{\left| \Phi_1 \right| - \left| \chi \right|}{\left| \Phi_2 \right| - \left| \chi \right|} \right)^{3/2}$$

(11)

From data measured on the Au- SAM-Au system we were able to estimate the barrier thickness, and the gold - molecule interface barrier height for both types of molecules.

For the Au-C11-Au samples we extract the Au-SAM interface barrier height as 2.1 eV, provided d=15 Å and Au-C16 interface barrier height as 2.0eV, provided d=19 Å. These values are close to metal - alkane SAM potential barriers obtained recently by various experiments. The low current conductivity measured on our systems is also in good agreement with values obtained on short chain alkanes. We found the ratio of Au-C11 potential barrier height to Au-C16 potential barrier height close to 1. This supports that tunneling proceeds primarily through σ-bonds of the alkane chains so that the barrier height is insensitive to chain length. Using alkanethiol molecules we tested the nanowires functionality and found that parameters (important for our devices functionality) of our molecules in nanowires were close to tabulated molecular parameters. So we were able to construct nanorods with different properties simply using different types of molecules. As in the case of alkanethiol self-assembled monolayers containing metal rods we prepared nanowires using replication inside the pores of 70 nm diameter polycarbonate track etch membranes. We integrated active molecules 4-[[2-nitro-4-(phenylethynyl) phenyl] ethynyl] benzenthiol into matrix of N-mercaptohexadecanoic acid molecules of the composition $HS(CH_2)_{15}COOH$ (they are referred below to as C_{16} molecules). The high affinity of Au to thiol groups results in a specifically oriented organic molecules. The height of 4-[[2-nitro-4-(phenylethynyl) phenyl] ethynyl] benzenthiol molecules molecules extends above the alkanethiol film so the top part of NDR molecules is in physical contact with gold deposited on C_{16} SAM. We again worked with nanowire that have a metal top contact, self-assembled monolayer (SAM) active region, and a metal bottom contact.
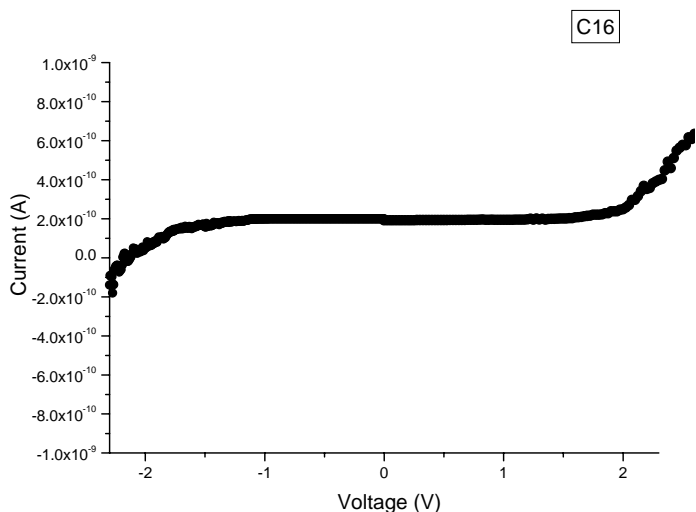
Fig. 2: Current versus voltage characteristics of the Au - C16 - Au structure in linear scale, over +1.3V to -1.3 V sweep.
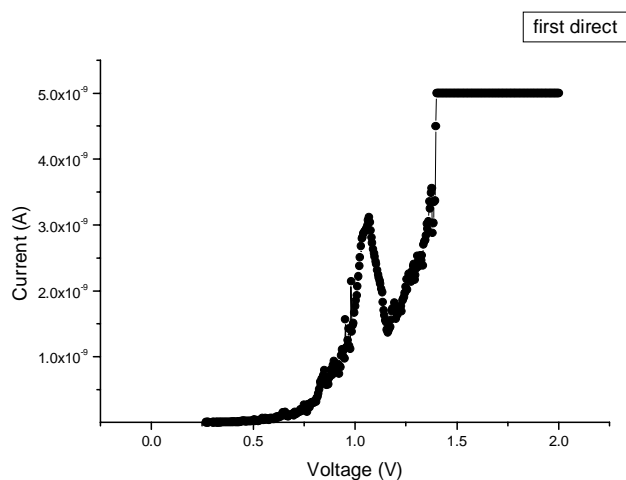

Fig.3: Current vs. voltage characteristics of Au-NDR-Au structure in linear scale in the range 0-2.5V.

NDR effect was clearly seen when positive bias (from 0 to 2.5 V) was applied to the system. The $I(V)$ curve was not fully reversible upon change of sweep direction (see Fig. 3). The NDR behaviour is absent in the control sample (containing just C_{16} molecules molecules, not 4-[[2-nitro-4-(phenylethynyl) phenyl] ethynyl] benzenthiol. The peak-to valley ratio in the case of positive

13

bias *I-V* curves is at room temperature 2.21, the position of the peak is at 1.068 V and peak current 3.12 10^{-9} A. The peak position is close to value previously obtained on similar systems at room temperature containing as active component the 4-[[2-nitro-4-(phenylethynyl) phenyl] ethynyl] benzenthiol molecules.

In order to explain the experimentally obtained characteristics we extended the previously published calculations [15, 16] examining Au bonded NDR and DR molecules and the influence of the static electric field plus charge variation. Typically for a self-assembled monolayer, one end of the molecule (usually consisting of a thiol group chemisorbed on a gold surface) has a strong contact, while the other end is physisorbed and has a weak contact. Therefore we model the entire setup consisting of molecule and contacting part of the electrode as a single super-molecule. Within this scheme the gold tips have been modeled by Au clusters. Due to the size of the whole supersystem three or four atomic Au_3 and Au_4 clusters have been used.

As a whole, the influence of the static electric field and charge variation were modeled for both systems. The interaction with the gold electrode influences the electronic structure of the NDR molecule nevertheless the main reason for the peak observed in *I-V* curves is associated with the fact that in self assembled monolayer containing NO_2, charge transfer occurs due to reduction from the chemically bonded end involving the level closest to the Fermi energy. This charge resides in a molecular orbital which, being partly occupied, lie close to the Fermi level. When charge is transferred and the MO closest to the Fermi level is occupied the main remaining electron transport through the molecule is tunneling so the level of the current drops down very rapidly. The overall picture can be influenced by the applied electric field.

III. Summary

We have established the formation of a metal/SAM/metal junctions inside nanowires through combined electroplating/electroless plating and template replication. Using alkanethiol molecules we tested the nanowires functionality and found that parameters of our molecules in nanowires were close to tabulated molecular parameters. On the molecular wires containing 4-[[2-nitro-4-(phenylethynyl) phenyl] ethynyl] benzenthiol molecules the current-voltage characteristics exhibited at room temperature negative differential resistance with on-off peak-to valley ratio 2.21. Thus novel method how to prepare nanostructure containing organic molecules with negative differential resistance (NDR) property has been worked out. We also demonstrated simple method

how to implement organic molecule into electronic circuit. We developed a method to form junctions containing self-assembled monolayers (SAM) of the organic molecules using the electric field self-assembly to place rod-shaped metal-SAM -metal nanowires from colloidal suspensions onto lithographically defined metal pads. So we have constructed electrical devices containing monolayer with NDR. We also modeled the influence of the static electric field and charge variation. The main reason for the peak observed in *I-V* curves is probably associated with the fact that in self assembled monolayer containing NO_2, charge transfer occurs due to reduction from the chemically bonded end involving the level closest to the Fermi energy.

IV. References

[1] M.A. Reed, C. Zhou, C.J. Muller, T.P. Burgin and J.M. Tour „Conductance of a molecular junction." Science, 278, 252-254, 1977.
[2]   L.A. Bumm et al „Are single molecular wires conducting?", Science, 271, 1705-1707, 1996.
[3] M.A. Reed, „Molecular –scale electronics", Proc. IEEE, 87, 652-658, Apr. 1999.
[4]   C. Zhou, M.R. Deshpande, M.A. Reed and J.M. Tour, „Nanoscale metal/self-assembled monolayer/metal heterostructures", Appl. Phys. Lett, vol. 71, 611-613, 1997.
[5] M.A. Ratner and J. Jortner, „Molecular electronics: Some directions" in Molecular Electronics, J. Jotner and M. Ratner, Eds. London, U.K. : Blackwell, 1997, 5-72, see also references cited therein.
[6] V. Mujica, M. Kemp and M.A. Ratner, „Electron conduction in molecular wires" , J. Chem. Phys., vol. 101, 6849-6855.
[7] Mbindyo J., Kovtyukhova N., Razavi B., Kratochvilova I., Angelo S., Mayer T., Jackson T., Mallouk T.: "Synthesis and assembly of nanowires for molecular electronics.", high-dielectric ceramics , 223, 155, 2002;
[8] J. K. N. Mbindyo, T. E. Mallouk, J. B. Mattzela, I. Kratochvílová, B. Razavi, T. N. Jackson, and T. S. Mayer: "Template Synthesis of Metal Nanowires Containing Monolayer Molecular Junctions", Journal of American Chemical Society, 124, 4020-4026, 2002.
[9] F. R.F. Fan, R.Y. Lai, J. Cornil, Y. Karzazi, J.L.Bredas, L.T. Cai, L. Cheng, Y.X. Yao, D.W. Price, S.M. Dirk, J.M. Tour, A.J. Bard, J. Am. Chem. Soc. 126, 2568, 2004.
[10] S. Záliš , I. Kratochvílová, A. Zambova, J. Mbindyo, T. E. Mallouk, T. S. Mayer : "Combined Experimental and Theoretical DFT Study of Molecular

Nanowires Negative Differential Resistance and Interaction With Gold Clusters.", EPJE, 18, 201, 2005.

 [11] M.A. Reed, C. Zhou, C.J. Muller, T.P. Burgin and J.M. Tour „Conductance of a molecular junction." Science, 278, 252-254, 1977.
[12] Balzani, V. ; Credi, A.; Raymo, F. M.; Stoddart, J. F. Angew. Chem. Int. Ed. 2000 39, 3349, 2000.
[13] Wong, E. W.; Collier, C. P.; Behloradsky, M.; Raymo, F. M.; Stoddart, J.F.; Heath, J.R. J. Am. Chem. Soc.122, 5831, 2000.
[14] Xu, T.; Peterson, I. R.; Lakshmikantham, M. V.; Metzger, R. M. Angew. Chem. Int. Ed. 40, 1749, 2001.
[15] J. M. Seminario, P. A. Derosa, J. L. Bastos, J. Am. Chem. Soc. 124, 10266, 2002.
[16] J. M. Seminario, A.G. Zacarias, P. A. Derosa, J. Phys. Chem. A 105, 791, 2001.

VI. Curriculum Vitae Ing. Irena Kratochvílová, Ph.D.

2.6. 1965 - born in Prague

Education and Qualifications:
1983-1989- MSc, Czech Technical University, Prague, thesis: „**Physical Models of the Solid State Micro - Systems**"
1990-1992 – Faculty of Mathematics and Physics, Charles University, Prague - neural network investigation with prof. Jiří Hořejš
1993 – 1998 - Ph.D. - Faculty of Nuclear Physics, Czech Technical University, Prague, thesis: "**Material Changes After Proton Impalnation into Dielectric Crystals**"

Professional Career:
1996-2004 – lectures for the MSc. students of the Faculty of the Nuclear Physics, Czech Technical University, Prague
Since 1997 – academic researcher – Group of Dielectric, Institute of Physics, Czech Academy of Sciences, Na Slovance 2, Prague 8, 182 21, Czech Republic
2001 – Penn State University – post-doc position - study of charge carrier transport through organic molecules, working on DARPA – funded project named "Direct Assembly of Molecular Logic Architectures Using Functionalized Metallic Nanowires", cooperation with teams from Penn State University, Rice University and Yale University.

Membership in Scientific Societies: Royal Chemical Society Associate editor
Amarican Material Research Society member

Research Areas and Interests:
- Ferroelectric Crystals Investigation,
- Investigation of isostructural glasses, crystals and glass-ceramic composites for optoelectronic applications.
- MFI Zeolites
- Molecular Nanosystems

Grant Projects Responsible Person
1999-2000 - GACR founded project "Investigation of isostructural glasses, crystals and glass-ceramic composites for optoelectronic applications. "
GAAV founded project A1040101/010/01 "Accesibility of the channel system in medium pore zeolites for molecules of aromatics. Computational simulation of the phenomenon. "
2001-2003 GACR fouded project 104/01/0945 " Possible application of light hydrocarbons separation by nano-leyers."
2005-07: GAAV funded project IAA400400501 "Coupling of diffusion flows in porous membranes and catalysts as studied by permeation and NMR techniques".
2001 - DARPA/ONR 98-1-0846 project : "Directed Assembly of Molecular Logic Architectures using Functiolalized Metallic Nanowires"
2001- US NAVY 01/9642 project: "Semiconductor Nanowires"
2006-2010 – COST project „Molecular photoconductive and photorefractive systems. From macro- scale towards nano-scale molecular electro- and photoresponsive devices"

Teaching Acitivies
1996-2006 – selected lectures for the MSc. students of the Faculty of the Nuclear Physics, Czech Technical University, Prague :
1996-1997   Theory of Algorithm
    1998-2000   Introduction to the Solid State Physics
    1998-2000   Physical Electronics
    2003-2006   Introduction to the Solid State Physics,

MSc. Work Leadership:
Baharak Razavi - Department of Electrical Engineering, Pennsylvania State University, USA, *Nanosystems Containing Organic Molecules*,
Brian Sosnowcik (Department of Civil Engineering), Pennsylvania State University, USA: *New Methods and Measurements in Modern Technologies*,

PhD. Students and Works Leadership:
Marco Cabassi (Cornell University), USA
James Matzella (Pennsylvania State University), USA
Chris Norquist (Pennsylvania State University), USA, *„Modern Trends in Electrical engineering"*
Martin Boldiš (VŠCHT Praha), Czech Republic– *„Simulation of nonisothermal sorption dynamics of the proces of bioethanol dewatering"*

Managing and Organizing Activities:
Nanolaboratory at Penn State with student team

Publications:
1 student textbook (coauthor), 90 positive citations in impacted scientific journals, main publications - see List of Selected Papers

List of Selected Papers:

J. Holakovský, I. Kratochvílová , M. Kočiřík: „A topological equivalence of percolation lattice for channel system in MFI type zeolites with that of diamond lattice", Microporous and Mesoporous Materials, 2006, 91 (1-3): 170-171.

Stanislav Záliš , Irena Kratochvilová, Jakub Šebera and Zdeněk Samec: *„DFT study of the interaction of organic molecules with gold clusters“*, CHIMIA, 2005, 7-8, P125;

S. Záliš, I. Kratochvílová, A. Zambova, J. Mbindyo, T. E. Mallouk, T. S. Mayer : “*Combined Experimental and Theoretical DFT Study of Molecular Nanowires Negative Differential Resistance and Interaction With Gold Clusters.*", Eur. Phys. J. E , 2005, 18, 201-206;

M. B. Smirnov, A. V. Menschikova, I. Kratochvílová-Hrubá and Z. Zikmund :   “*Lattice Dynamics and Phase Transition in LaBGeO$_5$",* phys. stat. sol. (b), 2004, 1-9;

I. Kratochvílová , M. Kočiřík, A. Zambova, J. Mbindyo, T. E. Mallouk, and T. S. Mayer: “*Room temperature negative differential resistence in molecular nanowires*", Journal of Materaterials Chemistry, 2002, **12**, 2927-2930;

I. Kratochvílová , A. Zambova, J. Mbindyo, B. Razavi, and J. Holakovský: “*Current-Voltage Characterization of Alkanethiol Self-Assembled Monolayers in Metal Nanowires. *", Modern Physics Letters B, 2002, **16**, 161-169;

Mbindyo J., Kovtyukhova N., Razavi B., Kratochvilova I., Angelo S., Mayer T., Jackson T., Mallouk T.: “Synthesis and assembly of nanowires for

19

molecular   electronics.“
high-dielectric ceramics , 2002, **223**, 155;

J. K. N. Mbindyo, T. E. Mallouk, J. B. Mattzela, I. Kratochvílová, B. Razavi, T. N. Jackson, and T. S. Mayer: *"Template Synthesis of Metal Nanowires Containing Monolayer Molecular Junctions"*, Journal of American Chemical Society, 2002, **124**, 4020-4026;

S. Evoy, B. Hailer, M. Duemling, W. Barnhart, S. Raman, B. R. Martin, T. E. Mallouk, I. Kratochvílová and T. S. Mayer: *"Hybrid Assembly of Nanoelectromechanical Systems"*, Material Research Society 2002-Proceedings, **676**, Y 322; 2002;

I. Kratochvílová-Hrubá , I. Gregora, J. Pokorný, S. Kamba, Z. Zikmund, J. Petzelt, M. Čerňanský, V. Studnička, V.N.Sigaev, E.N. Smelyanskaza: *"Vibrational spectroscopy of LaBSiO5 glass and glass-crystal composites"*, Journal of Non-Crystalline Solids, **290**, 224-230, 2001;

I. Kratochvílová, S. Kamba, I. Gregora, J Petyzelt, V.N. Sigaev, E.N. Smelyanskaya, V.I. Molev: *"Vibration properties of Pb5Ge3O11 and LaBGeO5 glasses and crystallised glasses."*, Ferroelectrics, **239**, 909-916, 2000 ;

I. Hrubá, S. Kamba, J. Petzelt, I. Gregora, Z. Zikmund, D. Ivannikov, G. Komandin, A. Volkov, B. Strukov: *"Optical phonons and ferroelectric phase transition in the LaBGeO5 crystal"*, physica status solidi (b), **214** , 423-439, 1999;

I. Hrubá, J. Král: „*Modification of LiNbO3 Optical Properties by He implantation*“, SPIE, **2967**, 180-185, 1996.