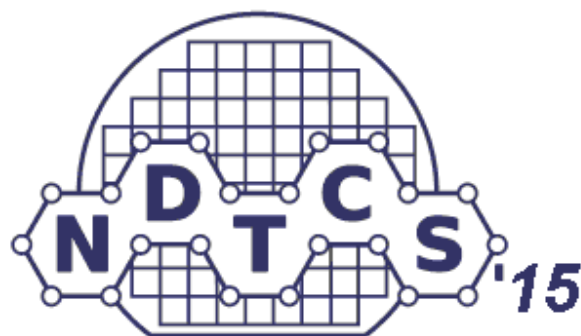


NANO-DESIGN, TECHNOLOGY, COMPUTER SIMULATIONS (NDTCS '15)

September 22-25, 2015

Program



GRODNO, BELARUS

NDTCS'2015 – September 22–25, 2015, Grodno, Belarus

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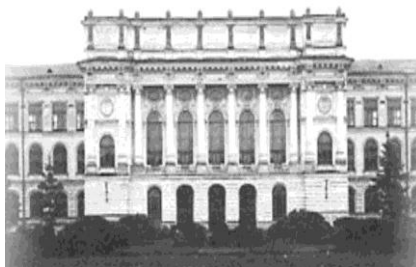
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IN COOPERATION WITH

The Ministry of Education of the Republic of Belarus



Yanka Kupala State University of
Grodno



St. Petersburg Academy
of Sciences for Strength Problems



Grodno House of Science and Technology

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NDTCS'2015 – September 22–25, 2015, Grodno, Belarus

FROM THE ORGANIZING COMMITTEE

We are proud to present the XVI International Workshop New Approaches to High-Tech: Nano-Design, Technology, Computer Simulations - NDTCS'2015. We welcome you to Grodno and hope, that you will find the conference professionally stimulating and personally enjoyable.

The NDTCS is organized regularly in various cities in the Europe and is one of the Central Europe's workshop in the field encompassing interdisciplinary research in nano-design, modern methods for structures and properties investigation of various nano-, micro- and macrosystems and computer simulation of physical and technological processes.

Starting from St. Petersburg in Russia more than 15 years of its history Workshop NDTCS has very changed and moved to the West. That allows organizing the effective science meetings for researchers from all over the world. In the last years NDTCS took place in Olsztyn, Poland (the X International Workshop, Joint Poland-Russia SPIE event, 2006), then in Bayreuth, Germany (the XI Workshop, 2007), in Minsk, Belarus (the XII Workshop, 2008), in Vilnius, Lithuania (the XIII Workshop, 2009), in Espoo, Finland (the XIV Workshop, 2011), in Minsk, Belarus (the XV Workshop, 2013). And now we are glad to meet you at the XVI Workshop here in Belarus.

All papers submitted to NDTCS'2015 have been reviewed and evaluated by minimum two members of the International Program Committee to put together a high quality technical program more than 50 papers organized in oral presentations. The NDTCS Organizing Committee would like to thank all reviewers for their hard work.

Therefore, we wish you successful discussions and a pleasant stay in Grodno!

NDTCS'2015 – September 22–25, 2015, Grodno, Belarus

GENERAL INFORMATION AND INQUIRES

Ph.D., Associate Professor Alexander Nikitin, co-chairman of
NDTCS'2015

Yanka Kupala State University of Grodno, Belarus

Department of Theoretical Physics and Thermal Engineering

Phone: +375 152 48 28 50 +375 152 48 50 11

Fax: +375 152 48 50 11

Post address: Belarus, Grodno, Gorkogo st., 72

E-mail: *nik@grsu.by*

Web: *http://belnts.by/*

TIMESTAMPS

The program of the NDTCS'2015 Workshop consists
invited lectures and original papers.

The time of presentations:

- for invited papers: 20-25 min. for presentation and 5-10 min. for questions
- for original papers: 10 min. for presentation and 5 min. for questions

REGISTRATION

Registration will take place in Grodno House of Science and
Technology (Belarus, Grodno, Gorkogo st., 72), lobby

GENERAL SCHEDULE

<u>DAY 1</u>	Tuesday, September 22, 2015
9:00	Registration
11:00	Conference Opening
11:30	Plenary Sessions
13:30	Lunch
14:30	Section 1
16:30	Coffee Break
17:00	Section 1 (<i>cont</i>)
18:00	Dinner

<u>DAY 2</u>	Wednesday, September 23, 2015
10:00	Section 2
11:00	Coffee Break
11:30	Section 2 (<i>cont</i>)
12.30	Lunch
13:30	Section 2 (<i>cont</i>)
14:30	Coffee Break
15:00	Section 2 (<i>cont</i>)
18:00	Social Program (Excursion)
21:00	Dinner

<u>DAY 3</u>	Thursday, September 24, 2015
10:00	Section 3
11:00	Coffee Break
11:30	Section 3 (<i>cont</i>)
13:00	Lunch
14:00	Section 3 (<i>cont</i>)
15:30	Coffee Break
16:00	Section 3 (<i>cont</i>)
17:30	Dinner

<u>DAY 4</u>	Friday, September 25, 2015
10:00	General Discussion and Closing Ceremony
12:00	Reception

PROGRAM OF THE CONFERENCE

TUESDAY, SEPTEMBER 22, 2015

INVITED LECTURES

- 1 THE SHORT DRAMATIC HISTORY OF NDTCS WORKSHOPS**
A. Melker
*Peter the Great Saint-Petersburg Polytechnic University SPBPU,
St. Petersburg, Russia*
- 2 GEOMETRIC AND PHYSICAL CHARACTERISTICS OF NANOOBJECTS**
V. Liopo
Yanka Kupala State University of Grodno, Grodno, Belarus
- 3 HIERARCHICAL APPROACH TO THE MODELING OF NANOSTRUCTURES**
V. Barkaline
Belarusian National Technical University, Minsk, Belarus
- 4 PETA RADIATION UNDER FIRST ORDER PHASE TRANSITIONS**
V. Tatartchenko
Saint-Gobain Crystals, France
- 5 COLLOIDAL NANO-OPTOELECTRONICS: STATE-OF-THE-ART AND PROSPECTIVES**
S. Gaponenko
B.I. Stepanov Institute of Physics NAS B

SECTION 1. SYNTHESIS, STRUCTURE AND PROPERTIES OF NANOMATERIALS (GRAPHENE, FULLERENES, NANOTUBES, NANOPARTICLES, COMPOSITES ETC.)

- 1.1** PLASMONIC GOLD FILMS PROVIDE PHOTOLUMINESCENCE OF CdSe/ZnS NANOCRYSTALS IN CONDITION OF STRONG EXCITON-PLASMON COUPLING
V. Askirka, T. Glebovich, I. Motevich, I. Sveklo, S. Maskevich, N. Strekal
Yanka Kupala State University of Grodno, Grodno, Belarus
- 1.2** COMPUTER GENERATION OF THE MODELS OF LOCALIZED DEFECTS OF CARBON NANOTUBES AND GRAPHENE
T. Grigorenko, V. Barkaline
Belarusian National Technical University, Minsk, Belarus
- 1.3** OPTICAL CHARACTERIZATION OF 3D DISPERSE SYSTEMS WITH NANO- AND MICRO- PARTICLES: MIXTURES
A. Bezrukova, O. Vlasova
Peter the Great Saint-Petersburg Polytechnic University SPBPU, St. Petersburg, Russia
- 1.4** EXPERIMENTAL STUDY OF ACTION OF RADIATION FORCES ON METAL NANOPARTICLES IN A LASER BEAM OF THE GAUSSIAN FORM
L. Gaida¹, E. Matuk¹, A. Afanas'ev², D. Guzatov¹
¹ *Yanka Kupala State University of Grodno, Grodno, Belarus*
² *B.I.Stepanov Institute of Physics, Minsk, Belarus*
- 1.5** STRUCTURE AND GRAPHS OF MIDI-FULLERENES
M. Krupina¹, A. Melker², S. Starovoitov¹, T. Vorobyeva¹
¹ *Department of Experimental Physics,*
² *Department of Mechanics and Control Processes*
Peter the Great Saint-Petersburg Polytechnic University SPBPU, St. Petersburg, Russia

- 1.6** INFLUENCE OF STRUCTURE AND PHASE COMPOSITION OF THE MATERIAL STEAM TURBINE BLADES FROM TITANIUM ALLOYS ON THEIR RESISTANCE TO EROSIIVE DESTRUCTION
N. Krylov, M. Skotnikova, G. Tsvetkova, G. Ivanov
Peter the Great Saint-Petersburg Polytechnic University SPBPU, St. Petersburg, Russia
- 1.7** THE FORM OF NANOCRYSTALS AND ATOMIC STRUCTURE OF THEIR SURFACES
V. Liopo, A. Nikitin, E. Ovchinnikov, A. Sabuts, A. Sitkevich
Yanka Kupala State University of Grodno, Grodno, Belarus
- 1.8** THE PHYSICAL PROPERTIES OF NANOPARTICLES
V. Liopo, A. Nikitin, E. Ovchinnikov, A. Sitkevich
Yanka Kupala State University of Grodno, Grodno, Belarus
- 1.9** POTENTIALS FOR ATOMIC-LEVEL COMPUTER SIMULATIONS
A. Lipnitskii, V. Savel'ev, I. Nelasov, A. Kartamyshev,
Belgorod State University, Belgorod, Russia
- 1.10** GROWTH OF MIDI-FULLERENES FROM TWENTY TO SIXTY
A. Melker
Peter the Great Saint-Petersburg Polytechnic University SPBPU, St. Petersburg, Russia
- 1.11** MECHANISMS OF LASER MODIFICATION IN THE TECHNOLOGY OF NANOCOMPOSITES AND METAL-POLYMER SYSTEMS
V. Sarokin¹, S. Avdeychik², V. Struk¹
¹*Yanka Kupala State University of Grodno, Grodno, Belarus*
²*"Molder" Ltd, Grodno, Belarus*
- 1.12** QUANTUM MECHANIC INVESTIGATIONS STABILITY OF THE CO₁₈O_N (N=1, 2, ...10) NANOPARTICLES
V. Skachkova¹, J. Tamuliene², V. Stempitsky¹
¹*Belarusian State University of Informatics and Radioelectronics, Minsk, Belarus*
²*Institute of Theoretical Physics and Astronomy of Vilnius University, Vilnius, Lithuania*

- 1.13** QUANTUM-CHEMICAL CALCULATIONS OF THE EXCITED STATE ENERGY DEPENDENCE ON TWISTING AND WAGGING COORDINATES IN THIOFLAVIN T
V. Stsiapura, S. Maskevich
Yanka Kupala State University of Grodno, Grodno, Belarus
- 1.14** APPROACH TO PARTITION SUM DERIVATION IN NON-ADDITIVE CASE, WITH USE OF SECONDARY QUANTISATION AND COMBINATORIAL COMPOSITIONS
Y. Tarasievich
Yanka Kupala State University of Grodno, Grodno, Belarus
- 1.15** MODELING NATURAL OSCILLATIONS THREE LAYER PLATE UNDER THE INFLUENCE OF THE IMPULSE LOADING
D. Trubenok, K. Kurochka
Sukhoi State Technical University of Gomel, Gomel, Belarus
- 1.16** PHOTOCROMIC NANOCOMPOSITES BASED ON DIARYLETHENES
G. Vasilyuk¹, S. Maskevich¹, D. Filimonenko², V. Yasinskii², I. Sveklo¹, A. Yaroshevich¹, V. Askirka¹, V. Barachevsky³, A. Ait³
¹*Yanka Kupala State University of Grodno, Grodno, Belarus*
²*B.I.Stepanov Institute of Physics, Minsk, Belarus*
³*RAS Photochemistry Center, Moscow, Russia*
- 1.17** INTERACTIONS BETWEEN C, N, O, H IMPURITIES AND VACANCIES IN HCP TI AND FCC AL FROM FIRST PRINCIPLES
Vo Duy Dat, A. Kartamyshev, A. Lipnitskii
Belgorod State University, Belgorod, Russia

WEDNESDAY, SEPTEMBER 23, 2015

**SECTION 2. APPLICATIONS OF NANOMATERIALS
(ELECTRONICS, MECHANICS, BIOLOGY ETC.)**

- 2.1** NUMERICAL METHODS OF CALCULATING HEAT CONDUCTIVITY OF FILLED POLYMERS
A. Bachurina¹, N. Babarika¹, A. Belko¹, A. Nikitin¹, L. Evseeva², S. Tanaeva²
¹ *Yanka Kupala State University of Grodno, Grodno, Belarus*
² *A.V. Luikov Heat and Mass Transfer Institute of the National Academy of Sciences of Belarus, Belarus*
- 2.2** SIMULATION OF ELECTROMECHANICAL PROPERTIES OF ORDERED CARBON NANOTUBE ARRAYS
V. Barkaline
Belarusian National Technical University, Minsk, Belarus
- 2.3** A QUANTUM CHEMICAL MODELING OF THE SORPTION OF THE Ni²⁺ IONS BY POLYURETHANE
E. Bobkova¹, M. Ksenofontov¹, L. Ostrovsckaja¹, A. Simbura², M. Shundalau¹
¹ *A.N. Sevchenko Institute of Applied Physical Problems at Belarusian State University, Minsk, Belarus*
² *Belarusian State University, Minsk, Belarus*
- 2.4** INVESTIGATION OF GEOMETRIC AND ELECTRONIC STRUCTURES OF HEUSLER ALLOYS: CUBIC AND TETRAGONAL LATTICE
T. Breczko¹, J. Tamuliene², R. Grechishkin³
¹ *University of Bialystok, Bialystok, Poland*
² *Vilnius University, Institute of Theoretical Physics and Astronomy, Vilnius, Lithuania*
³ *Tver State University, Tver, Russia*
- 2.5** MODELING OF TRI-O-ACETYLDENOSINE PREPOLYMERIZATION COMPLEXES IN SOLVENTS FOR MOLECULAR IMPRINTING PARAMETERS ESTIMATION
Ya. Douhaya, V. Barkaline
Belarusian National Technical University, Minsk, Belarus

- 2.6** QUANTUM-CHEMICAL MODELING OF SOME REACTIONS BETWEEN NONSTOICHIOMETRIC CLUSTERS Si_nO_m
N. Evstratov^{1,2}, I. Matyushkin^{1,2}
¹ *Moscow Institute of Physics and Technology, Russia, Moscow*
² *Molecular Electronics Research Institute, Russia, Moscow*
- 2.7** A REGULARIZATION OF THE NO-BOUNDARY WAVE FUNCTION
N. Gorobey, A. Lukyanenko
Peter the Great Saint-Petersburg Polytechnic University SPBPU, St. Petersburg, Russia
- 2.8** ON THE EQUATION OF STATE OF AN ANHARMONIC SOLID BODY
N. Gorobey, A. Lukyanenko
Peter the Great Saint-Petersburg Polytechnic University SPBPU, St. Petersburg, Russia
- 2.9** QUANTUM MECHANICAL MODELING OF AN ANION C60-PSEUDOPOTENTIAL.
V. Ivanov¹, R. Polozkov^{2,3}, I. Vrabel²
¹ *Peter the Great Saint-Petersburg Polytechnic University SPBPU, St. Petersburg, Russia*
² *ITMO University, St. Petersburg, Russia*
³ *Science Institute, University of Iceland, Reykjavik, Iceland*
- 2.10** NUMERICAL MODELING OF DONOR-BASED QUBIT STATES IN ELECTRIC AND MAGNETIC FIELDS
E. Levchuk, L. Makarenko
Belarusian State University, Minsk, Belarus
- 2.11** DISCRETE METHODS IN TECHNOLOGICAL DESIGN OF ReRAM CELLS: BY THE EXAMPLE OF CONDUCTING FILAMENT FORMATION IN NANOSCALE HfO_2
I. Matyushkin^{1,2}, G. Teplov^{1,2}, O. Orlov^{1,2}, N. Evstratov^{1,2}
¹ *Moscow Institute of Physics and Technology, Moscow, Russia*
² *Molecular Electronics Research Institute, Moscow, Russia*
- 2.12** STUDY OF Cu/Nb INTERFACE DIFFUSION BY MOLECULAR DYNAMICS SIMULATION
I. Nelasov, A. Lipnitskii
Belgorod State University, Belgorod, Russian Federation

- 2.13** INTEGRAL COMPUTER MODEL FOR SIMULATION OF STEELS HOT ROLLING ON MILL 2000 OF SEVERSTAL
A. Ogoltcov¹, D. Sokolov², S. Sokolov², A. Vasilyev²
¹Severstal Russian Steel, Cherepovets
²Peter the Great Saint-Petersburg Polytechnic University SPBPU, St. Petersburg, Russia
- 2.14** NONLINEAR MATHEU EQUATION IN QUANTUM LIMIT
A. Sanin, A. Smirnovsky
Peter the Great Saint-Petersburg Polytechnic University SPBPU, St. Petersburg, Russia
- 2.15** AB INITIO MULTI-REFERENCE PERTURBATION THEORY CALCULATIONS OF THE LOW-LYING STATES OF THE YBRB MOLECULE
M. Shundalau, A. Minko, I. Hlushakou
Belarusian State University, Minsk, Belarus
- 2.16** CALCULATIONS OF EFFICIENCY OF PHOTOCROMIC MOLECULAR TRANSFORMATIONS OF DIARYLETHENES ON SURFACE OF Au AND Ag NANOPARTICLES
G. Vasilyuk¹, A. Ait³, V. Barachevsky³, S. Maskevich¹, D. Filimonenko², V. Yasinskii², I. Sveklo¹, A. Yaroshevich¹, V. Askirka¹
¹Yanka Kupala State University of Grodno, Grodno, Belarus
²B.I. Stepanov Institute of Physics, Minsk, Belarus
³RAS Photochemistry Center, Moscow, Russia

THURSDAY, SEPTEMBER 24, 2015

SECTION 3. MOLECULAR DYNAMICS AND DFT SIMULATION

- 3.1** KINETICS AND FORMATION MECHANISMS OF NANOCOMPOSITE WEAR INHIBITORS OF METAL-POLYMER SYSTEMS
A. Antonov¹, S. Avdeychik², A. Vorontsov¹, G. Yuldasheva³
¹Yanka Kupala State University of Grodno, Grodno, Belarus
²«Molder» Ltd., Grodno, Belarus
³Tashkent Automobile and Roads Construction Institute, Tashkent, Uzbekistan

- 3.2** THE ENERGY FACTOR OF POLYMER NANOCOMPOSITES TECHNOLOGY
S. Avdeychik², V. Struk¹, Y. Eisymont¹, A. Ikramov³
¹*Yanka Kupala State University of Grodno, Grodno, Belarus*
²*«Molder» Ltd., Grodno, Belarus*
³*Tashkent Automobile and Roads Construction Institute, Tashkent, Uzbekistan*
- 3.3** EVALUATION OF LOCAL THERMAL STRESSES IN THE VICINITY OF FIBROUS AND PARTICULATE FILLERS IN THE COMPOSITE MATERIALS BASED ON FLUOROPOLYMERS
V.G. Barsukov¹, Y. Dahl², R. Lubovskaja¹, V.V. Barsukov³
¹*Yanka Kupala State University of Grodno, Grodno, Belarus*
²*Peter the Great Saint-Petersburg Polytechnic University SPBPU, St. Petersburg, Russia*
³*Grodno House of Science and Technology, Grodno, Belarus*
- 3.4** REVERSIBLE PLASTICITY AT THE STAGE OF RESIDUAL TWINNING
V. Bashmakov, T. Chikova
Yanka Kupala State University of Grodno, Grodno, Belarus
- 3.5** ON ENERGY DISSIPATION IN A FRICTION-CONTROLLED SLIDE OF A BODY EXCITED BY RANDOM MOTIONS OF A FOUNDATION
S. Berezin, O. Zayats
Peter the Great Saint-Petersburg Polytechnic University SPBPU, St. Petersburg, Russia
- 3.6** DIAGNOSTICS OF A CRATER GROWTH ON LASER PLASMA MATERIALS PROCESSING
A. Ivanov, A. Kapytski, N. Yarema, N. Zharkiy
Yanka Kupala State University of Grodno, Grodno, Belarus
- 3.7** INFLUENCE OF AN ELECTRIC FIELD ON NANOPARTICLES GENERATION DURING LASER PROCESSING OF METALS
A. Ivanov, A. Kapytski, S. Vasiliev
Yanka Kupala State University of Grodno, Grodno, Belarus
- 3.8** EVOLUTION OF NANOPARTICLES GENERATION ON LASER TREATING OF METALS IN LIQUID
A. Ivanov, A. Kapytski, S. Vasiliev
Yanka Kupala State University of Grodno, Grodno, Belarus

- 3.9** INTERACTION OF CLEAVAGE CRACK WITH SLIP BANDS IN LITHIUM FLUORIDE CRYSTALS
L. Karyev, A. Zanina, V. Feodorov
Tambov G.R. Derzhavin State University, Tambov, Russia
- 3.10** NONLINEAR VARIATIONAL PROBLEMS FOR ELASTIC MEDIUM WITH MICROSTRUCTURE
V. Lalin, E. Zdanchuk
Peter the Great Saint-Petersburg Polytechnic University SPBPU, St. Petersburg, Russia
- 3.11** THE ROLE OF DISPERSION EFFECTS AND DELAY FOR CONTINUUM MECHANICS
E. Prozorova
Peter the Great Saint-Petersburg Polytechnic University SPBPU, St. Petersburg, Russia
- 3.12** STRUCTURAL PRINCIPLES OF CREATING HIGHLY FILLED FLUORINE COMPOSITES
V. Sarokin¹, S. Avdeychik², A. Vorontsov¹, G. Yuldashev³, A. Ryskulov³
¹*Yanka Kupala State University of Grodno, Grodno, Belarus*
²*«Molder» Ltd., Grodno, Belarus*
³*Tashkent Automobile and Roads Construction Institute, Tashkent, Uzbekistan*
- 3.13** STANDARD PROGRAM FOR CALCULATING REFERENCE RADIOGRAPHS CRYSTALS
A. Senko, F. Sitkevich
Yanka Kupala State University of Grodno, Grodno, Belarus
- 3.14** TRIBOLOGICAL PROPERTIES OF LOW DENSITY PE FILLED WITH SILICA NANO PARTICLES
L. Shashura, I. Rouba
Grodno Branch «Research Center of Resources-Saving Problems» of A.V. Luikov Heat and Mass Transfer Institute of the National Academy of Sciences of Belarus

- 3.15** THE MECHANISM OF DEFORMATION OF GLASSY AND PARTIALLY CRYSTALLINE POLYMERS DURING THEIR STRETCHING IN THE SUPERCRITICAL FLUIDS
E. Trofimchuk¹, A. Efimov¹, N. Borisova², A. Dudnik¹, D. Bagrov¹, N. Nikonorova¹, L. Nikitin³
¹ *Moscow State University, Moscow, Russia*
² *Moscow State Pedagogical University, Moscow, Russia*
³ *Institute of Organoelement Compounds RAS, Moscow, Russia*
- 3.16** BIOMECHANICAL PROCESSES IN THE INTERVERTEBRAL CERVICAL DISK OF SPINE AT HIS MOTION
A. Zharnov¹, O. Zharnova²
¹ *Yanka Kupala State University of Grodno, Grodno, Belarus*
² *Grodno State Medical University, Grodno, Belarus*
- 3.17** FORMATION OF NANOSTRUCTURES ON THE SURFACE OF COPPER INDIUM GALLIUM SELENIDE THIN FILMS USING ARGON PLASMA ETCHING
D. Mokrov¹, S. Zimin¹, E. Gorlachev², I. Amirov², V. Naumov², V. Gremenok³, A. Pyatlitski⁴, T. Petliskaya⁴
¹ *Yaroslavl State University, Yaroslavl, Russia*
² *Yaroslavl Branch of the Institute of Physics and Technology of Russian Academy of Sciences, Yaroslavl, Russia*
³ *Scientific-Practical Materials Research Center of the NAS of Belarus, Minsk, Belarus*
⁴ *Belmicroanalysis State Center, RDC "Belmicrosystems" RPC "Integral", Minsk, Belarus*