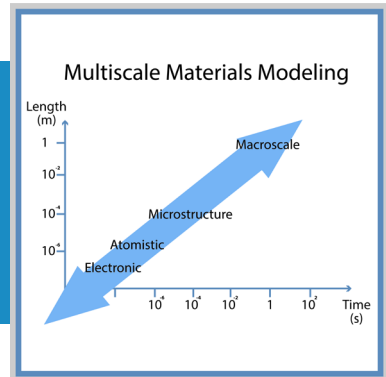


15–16  
October

International Association of Academies of Sciences  
Academy of Sciences of Belarus  
Department of Physicotechnical Sciences

PROGRAMME  
of International Workshop  
“Modeling of synthesis and  
destruction of advanced materials”



Minsk, BELARUS  
2018

## PROGRAMME

*of International Workshop*

### “MODELING OF SYNTHESIS AND DESTRUCTION OF ADVANCED MATERIALS”

**15–16 October 2018**

#### **Seminar venue:**

*Presidium of the National Academy of Sciences of Belarus (NASB),  
Conference Hall of the Presidium of NASB (room 216)  
66 Nezavisimosti Avenue, Minsk, Belarus*

*The working language of the Workshop is English.*

**15 October 2018**

**14:00–14:20**

EXPERIMENTAL NANOMECHANICS AND COMPUTER MODELING BASED ON SCANNING ELECTRON PROBE MICROSCOPY.

*S.A. Chizhik, Presidium of the National Academy of Sciences of Belarus and the A.V. Luikov Heat & Mass Transfer Institute, National Academy of Sciences of Belarus, Minsk.*

**14:20–14:40**

DFT-THERMODYNAMICS SIMULATION: ACCELERATOR OF FUNCTIONAL MATERIALS DEVELOPMENT.

*Heechae Choi, President, Materials Data Corp., Korea, and Group Leader, Institute of Inorganic Chemistry, University of Cologne, Germany,  
Eung-Kwan Lee, Volmi, Incheon, Korea.*

**14:40–15:00**

MODELING AND VERIFICATION OF SYNTHESIS OF SUPERHARD MATERIALS BASING ON PHYSICO-CHEMICAL NANOSTRUCTURAL ANALYSIS AND MULTIFRACTAL PARAMETRIZATION.

*P.A. Vityaz', Presidium of the National Academy of Sciences of Belarus, Minsk,  
M.L. Kheifetz, Presidium of the National Academy of Sciences of Belarus, Minsk,  
V.T. Senyut', Joint Institute of Mechanical Engineering, National Academy of Sciences of Belarus, Minsk, A.G. Kolmakov, The A.A. Baykov Institute of Metallurgy and Materials Science, Russian Academy of Sciences, Moscow, S.A. Klimenko, The V.N. Bakul' Institute of Superhard Materials, National Academy of Sciences of Ukraine, Kiev.*

**15:00–15:20**

MACROKINETIC MODELING OF DIFFUSION AND PHASE FORMATION DURING SYNTHESIS OF ADVANCED MATERIALS: COMBUSTION SYNTHESIS AND MECHANICAL ALLOYING.

*B.B. Khina, Physico-technical Institute, National Academy of Sciences of Belarus, Minsk.*

**15:20–15:40**  
**Coffee break**

**15:40–16:00**

TOPOLOGICAL SEMIMETALS: AB INITIO TIGHT-BINDING APPROXIMATION AND DFT-SIMULATION OF HFSIS BAND STRUCTURE.

H.V. Grushevskaya, N.N. Dorozhkin and G.G. Krylov, *Physics Department, Belarussian State University, Minsk.*

**16:00–16:20**

PREDICTION OF RESIDUAL STRESS IN AUSTENITIC STAINLESS STEEL CONSIDERING THE EFFECT OF PHASE TRANSITION.

Xiaoting Deng, *Institute of Metal Research, Chinese Academy of Sciences, Shenyang, People's Republic of China.*

**16:20–16:40**

DYNAMIC MODELING OF NUCLEATION AT FIRST-ORDER PHASE TRANSITION IN LANGMUIR MONOLAYER. APPLICATION TO FORMATION OF HEXAGONAL STRUCTURE.

N.G. Krylova, H.V. Grushevskaya and I.V. Lipnevich, *Physics Department, Belarussian State University, Minsk.*

**16:40–17:00**

OPTIMIZATION, SPECTROSCOPIC (FT–IR, EXCITED STATES, UV) STUDIES AND ELECTRONIC PROPERTIES OF NEW PYRIMIDINE AND AZOMETHINE DERIVATIVES.

Siyamak Shahab, *Institute of Physical Organic Chemistry, National Academy of Sciences of Belarus, and Belarussian State University, Minsk*, Masoom Sheikhi, *Young Researchers and Elite Club, Gorgan Branch, Islamic Azad University, Gorgan, Iran.*

**17:00–17:20**

MODELING OF DAMAGE ACCUMULATION IN METAL DURING ALTERNATING CYCLES OF FATIGUE LOADING.

A.A. Krechetov, *Kuzbass State Technical University, Kemerovo, Russia.*

**16 October 2018**

**10:00–13:00**

**Visiting the Scientific and Practical Center of NASB on Materials Science and The A.V.Luikov Heat & Mass Transfer Institute.**

GENERAL DISCUSSION.