

HOST INSTITUTE:

Khujand State University named after
Academician B. Gafurov
Ministry of Education and Science of the
Republic of Tajikistan



CO-ORGANIZERS:

Waseda University, Japan
Nagoya University, Japan
Keio University, Japan
Dubna University, Russia
S.U. Umavor PhTI, Tajikistan



- 10³⁰-11⁰⁰** **Coffee Break**
(Session VIII. Co-Chairs I. Ghosh & A. Kuznetsov)
- 11⁰⁰-11³⁰** **Subrata Majumder** (N.I.T., Patna, India).
“Effect of surface modification of TiO₂ on conformational changes of DNA structure: experimental and theoretical studies”
- 11³⁰-12⁰⁰** **Kholmurzo Kholmurodov** (JINR, Dubna, Russia).
“Molecular dynamics modelling of nucleotides, peptides & DNA interactions with CNT & TiO₂ surfaces”
- 12⁰⁰-12³⁰** **Tatyana Zelenyak** (Dubna State University, Dubna, Russia).
“The experimental and molecular dynamics simulation studies of hybrid perovskite structures”
- 12³⁰-13⁰⁰** **Zarif Sharipov** (JINR, Dubna, Russia).
“Continuously-atomistic simulation of physical processes in metals under irradiation with high-energy heavy ions”.
- 13⁰⁰-14³⁰** **Lunch**
(Session IX. Co-Chairs G. Riznichenko & S. Majumdar)
- 14³⁰-15⁰⁰** **Ilya Kovalenko** (Moscow State University, Russia)
“Plastocyanin and cytochrome f protein-protein complex formation: simulation of binding mechanism”.
- 15⁰⁰-15³⁰** **Khikmat Muminov** (S.U.Umarov PhTI, AS RT, Dushanbe, Tajikistan).
“Interactions of topological vortexes with domain wall in 2D O(3) nonlinear σ -model”.
- 15³⁰-16⁰⁰** **Alimakhmad Kholov** (S.U.Umarov PhTI, AS RT, Dushanbe, Tajikistan)
“Dielectrical properties of cesium molybdenum monocrystals”
- 16⁰⁰-16³⁰** **Coffee Break**
(Session X. Co-Chairs Kh. Kholmurodov & Kh. Muminov)
- 16³⁰-17⁰⁰** **Sabur Abdullaev** (S.U. Umarov PhTI AS RT, Dushanbe, Tajikistan).
“Aerosol pollution atmosphere on result of the dust storms (dust haze) and its influence on climate change”.
- 17⁰⁰-17³⁰** **Sh.Kurbanbaev** (Inst. Ion-Plasma and Laser Technologies, Tashkent, Uzbekistan).
“Heat conductivity of thin-disperse porous mixtures”.
- 17³⁰-18⁰⁰** **Kh.Tilloboev** (Khujand State University, Khujand, Tajikistan).
“Chemical and radioactive compound as danger factors to health organism”.
- 18⁰⁰-18³⁰** **A. Leksovskii** (Khujand Science Center, Khujand, Tajikistan).
“The influence of thermocycle on process of adhesion contact”.
- 18³⁰-19⁰⁰**

September 28, Wednesday

Half-Day scientific program: 09⁰⁰-12⁰⁰
(Reserved speakers: Khatam Murtazaev;
other local and international speakers)
Symposium Closing.

**Khujand State University named after
Academician B. Gafurov, Ministry of
Education and Science of the Republic
of Tajikistan**

&

**Joint Institute for Nuclear Research
Dubna, Moscow region, Russia**

INTERNATIONAL SYMPOSIUM

KSCMBS'16

**“Khujand Symposium on
Computational Materials
and Biological Sciences”**

**24-28 September 2016
Khujand State University
named after
Academician B. Gafurov
Khujand, Tajikistan**

SCIENTIFIC PROGRAM



INTERNATIONAL SYMPOSIUM KSCMBS'16

September 24, Saturday

Arrival in Khujand, Tajikistan.

September 25, Sunday (Hotel "Bahoriston" & Khujand State University named after Academician B. Gafurov)

08⁰⁰-08³⁰ Registration in Hotel "Bahoriston".
08³⁰-09⁰⁰ Opening ceremony. Welcoming by Rector of Khujand State University named after Academician B. Gafurov, by Governmental Representatives and Academy of Sciences of the Republic of Tajikistan.

(Session I. Co-Chairs Kh.Kholmurodov & A.Maqsudov)

09⁰⁰-09³⁰ Mitsuhiro Matsumoto (Kyoto University, Japan).
"Mesoscale modelling for lubrication mechanism of human joints"
09³⁰-10⁰⁰ Genri Norman (JIHT, RAS, Moscow, Russia).
"Plasma phase transition in warm dense hydrogen"
10⁰⁰-10³⁰ Tomobe Katsufumi (Keio University, Japan).
"Molecular dynamics simulation of Rhodopsin and Opsin: Water transport through internal water pathways"

10³⁰-11⁰⁰ Coffee Break

(Session II. Co-Chairs G. Norman & M. Khojaeva)

11⁰⁰-11³⁰ Pavel Volynsky (Shemyakin-Ovchinnikov IBCh, Russia).
"Thermal sensitivity of TRPV1 receptor as probed by computer simulations"
11³⁰-12⁰⁰ Vasily Pisarev (JIHT, RAS, Moscow, Russia).
"Molecular dynamics simulations of gas condensate mixture in porous medium"
12⁰⁰-12³⁰ Takashi Ao (Kyoto University, Japan).
"MD simulation of sandwiched liquid evaporation"
12³⁰-13⁰⁰ Daria Pyrkova (Shemyakin-Ovchinnikov IBCh, Russia).
"How force field affects the properties of two-component lipid bilayers: a molecular dynamics study"

13⁰⁰-14³⁰ Lunch

14³⁰-18⁰⁰ Visiting Faculty of Physics of Khujand State University and Khujand city.

September 26, Monday (Hotel "Bahoriston" & Khujand State University named after Academician B. Gafurov)

09⁰⁰-10³⁰ (Session III. Co-Chairs A. Maqsudov & Kh.Kholmurodov)
Khujand State University named after Academician B. Gafurov.
Short (very general) presentations by all keynote speakers. Discussions with Tajikistani students on education-science topics.

10³⁰-11⁰⁰ Coffee Break

11⁰⁰-11³⁰

(Session IV. Co-Chairs M. Matsumoto & P. Volynsky)
Roman Efremov (Shemyakin-Ovchinnikov IBCh, Russia).
"Stochastic but fine-tuned: dualism in cell membranes' organization as revealed by computer simulations"

11³⁰-12⁰⁰

Tomoyuki Yamamoto (Waseda University, Japan).
"Origin of room temperature ferromagnetism in dilute magnetic oxides"

12⁰⁰-12³⁰

Andrey Kuznetsov (Shemyakin-Ovchinnikov IBCh, RAS).
"Helix-helix interactions in membranes: focus on lipids"

12³⁰-13⁰⁰

Takuma Nozawa (Keio University, Japan).
"Coarse-grained simulations to investigate the phase behavior of chiral liquid crystals"

13⁰⁰-14³⁰

Lunch

14³⁰-15⁰⁰

(Session V. Co-Chairs T. Yamamoto & R. Nazarov)
Siewert Jan Marrink (University of Groningen, Netherlands).

15⁰⁰-15³⁰

"Computational microscopy of cellular membranes"
Maxim Orekhov (JIHT, RAS, Moscow, Russia).
"Ion dynamics and ion solvation. Water and Lennard-Jones liquid"

15³⁰-16⁰⁰

Shinjiro Nakamura (Keio University, Japan).
"Vibrational spectra analysis of water molecules in infrared region using anharmonic potential"

16⁰⁰-16³⁰

Coffee Break

16³⁰-17⁰⁰

(Session VI. Co-Chairs D. Pyrkova & T. Nozawa)

17⁰⁰-17³⁰

Indira Ghosh (JNU, Delhi, India)
"Designing of Antimalarial compounds using MD simulation"

17³⁰-18⁰⁰

Sanhita Majumdar (IEST, West Bengal, India)
"Wet Chemical Synthesis of Reduced Graphene Oxide and its Appl. in Gas Sensor, Humidity Detector and Solar Cell"
Armen Poghosyan (NAS, Yerevan, Armenia).

18⁰⁰-18³⁰

"Frequency dependence scaling on K40 GPU. A GROMACS benchmarking"

19⁰⁰-21⁰⁰

Elena Kirova (JIHT, RAS, Moscow, Russia)
"Glass transition process at Al melt cooling"

Welcome Party

September 27, Tuesday (Hotel "Bahoriston" & Khujand State University named after Academician B. Gafurov)

09⁰⁰-09³⁰

(Session VII. Co-Chairs R. Efremov & T. Katsufumi)
Galina Rznichenko (Moscow State University, Russia).
"Kinetic and comp. model. of photosynthetic regulation"

09³⁰-10⁰⁰

Dmitry Nolde (Shemyakin-Ovchinnikov IBCh, Russia).
"Performance optimization of GROMACS software on modern computers"

10⁰⁰-10³⁰

Nikolay Kondratyuk (JIHT, RAS, Moscow, Russia).
"Consistent mol. dynamics calculation of diffusion in higher n-alkanes"

