

HOST INSTITUTE:

S.U.Umarov Physical-Technical Institute,
Academy of Sciences of Republic of
Tajikistan



CO-ORGANIZATORS:

Waseda University, Japan
Nagoya University, Japan
Keio University, Japan
Dubna University, Russia



- 13³⁰-14⁰⁰ **(Session VIII. Co-Chairs R. Efremov & A. Chugunov)**
Aram Shahinyan (Int.Sci.-Edu.Center, NAS, Armenia)
"Mechanism of interaction of macromolecules with surfactant micelles in aqueous solution: a molecular dynamics simulation"
14⁰⁰-14³⁰ **Kholmirzo Kholmurodov** (JINR, Dubna, Russia).
"Molecular dynamics modeling of DNA photolyase enzyme for the UV-induced DNA damages"
Roman Eremin (JINR, Dubna, Russia).
"Oleic acid in benzene and decalin: Solvation shell effect on small-angle neutron scattering"
Eric Dushanov JINR, Dubna, Russia).
"Difference of behavior of DNA and CPD in the repairing molecular systeme".
Mirzoaziz Khusenov(MoscowSt.Univ.Tech. "STANKIN")
"MD simulation of DNA-CNT interaction processes".
14³⁰-15⁰⁰ **Zafari Umar** (Tomsk State Pedagogical Univ., Russia)
"The electron structure of MgO@64 single well nanotube"
15⁰⁰-15²⁰ **Coffee Break**
(Session IX. Co-Chairs Kh.Kholmurodov & Kh.Muminov)
15²⁰-15⁵⁰ **Ilnur Saitov** (JIHT, RAS, Moscow, Russia).
"Dielectric properties of warm dense matter".
15⁵⁰-16²⁰ **Farshed Karimov** (The Institute of Geology, Earthquake Engineering and Seismology of the AS RT, Tajikistan).
"Some models for the magnetic properties of biological micro objects in the Earth magnetic field (metatactic spirillum bacteria)".
16²⁰-16⁵⁰ **Grigory Smirnov** (JIHT, RAS, Moscow, Russia).
"Phase diagram of methane and hydrogen hydrates from atomistic modeling"
16⁵⁰-17²⁰ **Alexei Shvetsov** (Nucl.Phys.Inst., NRC"Kurchatov Institute").
"To be announced".
17²⁰-17⁵⁰ **Georgy Rychkov**(Nucl.Phys.Inst., NRC"Kurchatov Institute").
"To be announced".
18⁰⁰-18³⁰ **Coffee Break. Discussions with Tajikistani scientists at PhTI Laboratories.**

September 27, Saturday
(Sightseeing around Dushanbe)

September 28, Sunday
(Closing.Returning back from Dushnbe to Moscow)

**S.U.Umarov Physical-Technical
Institute, Academy of Sciences of
Republic of Tajikistan**

&

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

**1st International Symposium
DSCMBS'14
"Dushanbe Symposium on
Computational Materials
and Biological Sciences"**

**INTERNATIONAL
SYMPOSIUM**

**23-28 September 2014
S.U.Umarov PhTI
Dushanbe, Tajikistan**

**SCIENTIFIC
PROGRAM**

SCIENTIFIC PROGRAM



INTERNATIONAL SYMPOSIUM

September 23, Tuesday

Arrival in Dushanbe, Tajikistan.

September 24, Wednesday (S.U.Umarov PhTI, Dushanbe, Tajikistan)

- 09⁰⁰-09³⁰ **Opening ceremony. Welcoming by President of Academy of Sciences of the Republic of Tajikistan, by Director of the S.U.Umarov PhTI, by Governmental Representatives.**
(Session I. Co-Chairs Kh Kholmurodov & Kh.Muminov)
Academician Mikhail Ostrovsky (Emanuel Institute of Biochemical Physics, RAS, Moscow).
“Visual pigment rhodopsin: structure, photochemistry, functions”
- 09³⁰-10⁰⁰ **Yuko Okamoto** (Nagoya University, Japan).
“Generalized-ensemble algorithms for materials and biological sciences”
- 10⁰⁰-10³⁰ **Coffee Break**
(Session II. Co-Chairs K.Yasuoka & T.Feldman)
- 10³⁰-10⁵⁰ **Takao Yoda** (Nagahama Inst. Bio-Sci. & Tech., Japan).
“Simulation Study on Conformation Distributions of Small Peptides”
- 10⁵⁰-11²⁰ **Roman Efremov** (Shemyakin-Ovchinnikov IBCh, Russia).
“Biological membranes as structural/dynamic template for new nanomaterials: insights from computer simulations”
- 11²⁰-11⁵⁰ **Viktor Lakhno** (Inst.Math.Prob.Bio.,Pushchino, Russia).
“Charge transfer by nonlinear excitations in DNA”
- 11⁵⁰-12²⁰ **Lunch**
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- 12²⁰-13³⁰ **(Session III. Co-Chairs T. Yamamoto & A. Kuznetsov)**
Catherine Etchebest (University Paris-Diderot, France).
“New control mechanisms of water transport identified in AQP1 by combining molecular dynamics simulations and experiments”.
- 13³⁰-14⁰⁰ **Kenji Yasuoka** (Keio University, Japan).
“Molecular dynamics simulations of lipid bilayer”
- 14⁰⁰-14³⁰ **Tomobe Katsufumi** (Keio University, Japan).
“To be announced”
- 14³⁰-15⁰⁰ **Coffee Break**
(Session IV. Co-Chairs T. Yoda & T. Salikhov)
- 15⁰⁰-15²⁰ **Tomoyuki Yamamoto** (Waseda University, Japan).
“Electronic structure analysis of functional materials by synchrotron radiations and first-principles calculations”.
- 15²⁰-15⁵⁰ **Mitsuhiro Matsumoto** (Kyoto University, Japan).
“Lubrication mechanism in joints – Role of biopolymers”
- 15⁵⁰-16²⁰ **Donguk Suh** (Keio University, Japan).
“Simulations of Vapor-to-Liquid Nucleation on Various Solid Precursor Particle Configurations by Molecular Dynamics”
- 16²⁰-16⁵⁰ **Genri Norman** (JIHT, RAS, Moscow, Russia).
“Plasma-plasma and melt-melt first-order phase transitions”
- 16⁵⁰-17²⁰ **Academician Rahim Marupov** (S.U.Umarov PhTI, Tajikistan).
“To be announced”
- 17²⁰-17⁵⁰ **Welcome Party**
- 18⁰⁰-20⁰⁰

September 25, Thursday
(Meetings at National University of Tajikistan)

- 10⁰⁰-12²⁰ **(Session V. Co-Chairs Kh.Kholmurodov & Kh.Muminov)**
Short (very general) presentations by all keynote speakers for the Tajikistani students
- 12²⁰-13³⁰ **Lunch**
- 13³⁰-15⁰⁰ **Sightseeing of Tajik National Museum (Great Wooden Statue of Buddha of ancient Central Asia, etc)**
- 15⁰⁰-18⁰⁰ **Sightseeing of mountain river Varzob**

September 26, Friday (S.U.Umarov PhTI, Dushanbe, Tajikistan)

- 09⁰⁰-09³⁰ **(Session VI. Co-Chairs Kh.Kholmurodov & Kh.Muminov)**
Vladimir Stegailov (JIHT, RAS, Moscow, Russia).
“Graphite melting: atomistic kinetics resolves long-standing controversy”
- 09³⁰-10⁰⁰ **Tatiana Feldman** (Lomonosov Moscow State University).
“Visual pigment rhodopsin as a concept for ultrafast optical molecular switch creation”
- 10⁰⁰-10³⁰ **Andrei Kuznetsov** (Moscow Inst.Phys. & Tech., Russia).
“The adaptable lipid matrix promotes transmembrane helices association in membranes”
- 10³⁰-10⁵⁰ **Coffee Break**
(Session VII. Co-Chairs G. Norman & V. Stegailov)
- 10⁵⁰-11²⁰ **Anton Chugunov** (Shemyakin-Ovchinnikov IBCh, Russia).
“Liquid but durable: atomistic computer simulations explain unique properties of archaeal-like membranes”
- 11²⁰-11⁵⁰ **D.E.Nolde** (Shemyakin-Ovchinnikov IBCh, Russia).
“Molecular dynamics study of lipid-II in bacterial membranes”.
- 11⁵⁰-12²⁰ **Kikmat Muminov** (S.U.Umarov PhTI, Tajikistan).
“To be announced”.
- 12²⁰-13³⁰ **Lunch**