

MSSMBS'10

International Workshop MSSMBS 2010: Preliminary Program

September 26

Arrival and Registration in "Dubna" hotel

September 27

- 09³⁰–10⁰⁰ **Opening ceremony**. Welcoming by JINR Directorate.
- 10⁰⁰–10⁴⁵ **Tomoyuki Yamamoto** (Waseda University, Japan). "Local environment analysis of dilute dopant in functional materials by using the synchrotron radiation and the first principles calculation" .
- 10⁴⁵–11³⁰ **Roman Efremov** (Shemyakin–Ovchinnikov Institute of Bioorganic Chemistry, RAS, Moscow). "Lateral heterogeneity as an intrinsic property of hydrated lipid bilayers: a molecular dynamics study".
- 11³⁰–11⁴⁵ **Coffee Break**
- 11⁴⁵–12³⁰ **Viktor Lakhno** (IMPB, Pushchino Scientific Center, RAS). "Nano- and bio-electronics – possible solution ways, simulation approach".
- 12³⁰–13¹⁵ **Yulia Novakovskaya** (MSU, Russia). "Modelling small water clusters as a source of information about some characteristics of nanoscale systems".
- 13¹⁵–14¹⁵ **Lunch**
- 14¹⁵–15⁰⁰ **Kenji Yasuoka** (Keio University, Japan). "MD simulations and GPU Video-Game computers" (to be announced).
- 15⁰⁰–15⁴⁵ **Leonid Chernozatonskii** (Emmanuel Institute of Biochemical Physics, RAS, Moscow). "Graphene-graphane mixing nanostructures: hydrogen functionalization of graphene, properties and applications".
- 15⁴⁵–16⁰⁰ **Coffee Break**
- 16⁰⁰–16⁴⁵ **Aram Shahinyan** (The Institute of Applied Problems of Physics, NAS, Armenia, Erevan). "Molecular dynamics study of the human red blood cells".
- 16⁴⁵–17³⁰ **Genri Norman** (Joint Institute for High Temperatures, RAS, Moscow). "Atomistic theory of nucleation in solids and liquids" .
- 17³⁰–18¹⁵ **Vladimir Stegailov** (Joint Institute for High Temperatures, RAS, Moscow). "Ab initio models of electron subsystem response on external perturbations in molecules, liquids

and solids ”.

- 18¹⁵–19⁰⁰ **Pavel Volynsky** (Shemyakin–Ovchinnikov Institute of Bioorganic Chemistry RAS, Moscow). “Prediction and characterization of transmembrane helical dimers using computer simulation techniques”.
- 13¹⁵–19⁰⁰ **Poster and short communications:**
Ermuhammad Dushanov (LIT, JINR & INP, UzbRep), Kholmirzo Kholmurodov (LRB, JINR), Vladimir Korenkov (LIT, JINR), Mikhail Altaisky (LRB, JINR), M Murakami (Keio Univ. & Sony Corporation, Japan), M Yonekawa (Keio Univ., Japan), Viktor Krylov (LRB, JINR), Natalia Koltovaya (LRB, JINR), Guzel Aru (LRB, JINR), Oleg Belov (LRB, JINR) ...
- 19¹⁵ **Welcome Party**

September 28 (moving from JINR, Dubna to MSU, Moscow)

- 11⁰⁰–11⁴⁵ **Yuko Okamoto** (Nagoya University, Japan). “Generalized–ensemble simulations in protein science”.
- 11⁴⁵–12³⁰ **Alexander Nemukhin** (MSU, Russia). “Modeling structure and spectra of photoreceptor proteins”.
- 12³⁰–14⁰⁰ **Lunch**
- 14⁰⁰–14⁴⁵ **Fuyuki Shimojo** (Kumamoto University, Japan). “to be announced”.
- 14⁴⁵–15¹⁰ **Anton Polyansky** (Shemyakin–Ovchinnikov Institute of Bioorganic Chemistry RAS, Moscow). “Applications of surface hydrophobicity analysis for peptides, proteins and membranes”.
- 15¹⁰–15³⁵ **Anton Chugunov** (Shemyakin–Ovchinnikov Institute of Bioorganic Chemistry RAS, Moscow). “Mining of structural regularities in transmembrane domains of proteins: advantage for structure prediction”.
- 15³⁵–16⁰⁰ **A.A. Artyukh** (Emmanuel Institute of Biochemical Physics, RAS, Moscow). “Mechanic properties of graphene ribbon–carbon nanotube nanostructures ”.
- 16⁰⁰–16¹⁰ **Coffee Break**
- 16¹⁰–16³⁵ **K.V. Bertz** (Emmanuel Institute of Biochemical Physics, RAS, Moscow). “Structure and mechanic properties of chiral Si–nanowires”.
- 16³⁵–17²⁰ **Alexander Moskovsky** (MSU) “Computational chemistry applications of SKIF supercomputers ”.
- 17²⁰–18⁰⁵ **Kholmirzo Kholmurodov** (LRB, JINR) “Molecular dynamics studies on protein mutant and material science models”.
- 12³⁰–18⁰⁵ **Poster and short communications**
- 18⁰⁵–18³⁰ **Round table. Concluding remarks. Closing**
- 18³⁰ **Excursion to Chemistry Department and MSU. (returning from Moscow to Dubna)**