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
- 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".

- **1805–1830 Poster and short communications**

- **1830 Round table. Concluding remarks. Closing**

- **1830 Excursion to Chemistry Department and MSU. (returning from Moscow to Dubna)**