

COMPUTER DESIGN FOR NEW DRUGS AND MATERIALS

MOLECULAR DYNAMICS OF NANOSCALE PHENOMENA

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(Editor)

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ORGANIZING COMMITTEE: Anvar Maqsudi (Co-Chairman, Khujand State University, Tajikistan), Kholmurzo Kholmurodov (Co-Chairman, JINR, Russian Federation), Kenji Yasuoka (Co-Chairman, Keio University, Japan), Roman Efremov (Co-Chairman, IBCh, Russian Federation), Tomoyuki Yamamoto (Co-Chairman, Waseda University, Japan), Yuko Okamoto (Co-Chairman, Nagoya University, Japan)

ORGANIZED BY: Khujand State University of The Ministry of Education and Science of The Republic of Tajikistan and The Joint Institute for Nuclear Research of Russian Federation

TOPICS COVERED:

- Computer molecular simulation methods and approaches
- Molecular dynamics (MD) and Monte-Carlo (MC) techniques
- Modeling of biological molecules (RNA, DNA, proteins, enzymes, mutation transitions, etc.)
- Radiation physics, the impact of radiation on the biosphere, solid state physics (condensed matter physics)
- Physical and biochemical systems (gasses, crystals, liquids, polymers, bio-tribology, etc.)
- Material fabrication and design (ion doped structures, high pressure clathrates, carbon nanotubes)
- Drug design in medicine (docking of one molecule to another, inhibitory activities of enzymes)
- Computational and computing physics, chemistry, biology and medicine
- GPU accelerated molecular dynamics & related techniques

THE PRINCIPAL AIMS: We provide a platform for computer molecular simulation communities and scientists working in the material and biological areas to meet and share thoughts on latest trends. The main objective is to focus on the molecular dynamics simulations of chemical physics and biophysical systems.

LIST OF CO-SPONSORS:

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



Joint Photos of the International Symposium KSCMBS-2016
"Khujand Symposium on Computational Materials and Biological Sciences"
(At the conference hall and near Tajik national "Chaykhane" of the "Bahoriston" hotel)



The Photos of the KSCMBS'16 International Symposium

Contents

Preface	vi
Computer Design for New Drugs and Materials <i>Molecular Dynamics of Nanoscale Phenomena:</i> An Introduction	ix
Chapter 1. Computational Microscopy of Mitochondrial Membranes	1
Bibliography	12
Chapter 2. Integrative Method for Finding Antimalarials Using <i>In Silico</i> approach	13
Bibliography	38
Chapter 3. Mesoscale Modelling for Lubrication Mechanism of Human Joints	43
Bibliography	52
Chapter 4. How Force Field Affects the Properties of Two-Component Lipid Bilayers	53
Bibliography	63
Chapter 5. Molecular Basis of Protein-Protein Interactions in Membranes: A Computational Investigation	65
Bibliography	74
Chapter 6. MD Simulation of Sandwiched Liquid Evaporation	79
Bibliography	89
Chapter 7. Molecular Dynamics Simulations of Hybrid Halide Perovskites: The Effect of Bond Rigidness and Heating on the Structural Properties	91
Bibliography	117
Chapter 8. Pyrimidine-Purine and CPD-Purine Interactions in DNA Repairing Process	119
Bibliography	127
Chapter 9. Nonlinear Dynamic Properties of One-dimensional Anisotropic Heisenberg Ferromagnetic	129
Bibliography	137

Chapter 10. Modelling of Nonequilibrium Chemo-Electronic Conversion of Water Adsorption on the Surface of Yttria-Stabilized Zirconia: Experimental Preparation and Problem Overview	139
Bibliography	149
Chapter 11. Brownian Dynamics Study of Complex Formation of Proteins Plastocyanin and Cytochrome <i>f</i>	151
Bibliography	162
Chapter 12. X-Ray Absorption Near-Edge Structure Measurements and First-Principles Density Functional Theory Calculations for Local Environment Analysis of Trace Elements in Bioceramics	163
Bibliography	174
Index	175

Preface

In this book, the original papers have been collected that demonstrate the efficient use of the computer molecular dynamics (MD) simulation methods for the studying of nanoscale phenomena in the materials and life sciences. This volume contains the Proceedings of the International Symposium KSCMBS-2016 "Khujand Symposium on Computational Materials and Biological Sciences" (10th Japan–Russia Workshop "Molecular Simulation Studies in Materials and Biological Sciences"), which have been organized by the Joint Institute for Nuclear Research (JINR, Dubna) and Khujand State University named after Academician B. Gafurov, The Ministry of Education and Science of The Republic of Tajikistan (HGU, *hgu.tj*, RT) during the September 24–28, 2016 in Khujand, Tajikistan.

One has to mention that the Japan-Russia International Workshop MSSMBS with active participation of European, USA, Canadian, etc., scientists and research groups has already been held five times during 2004-2012 at JINR (the 5th MSSMBS workshop was held on the base of JINR of Dubna on 9-12 September 2012). Also during 10-12 September 2013-2015 in Japan the 1st and 2nd International Symposiums on Computational Materials and Biological Sciences were held in Waseda and Nagoya Universities, that make the bilateral collaboration more international. Thus, the border of the scientific cooperative meeting on the world scale has greatly been expanded, with a hope that the KSCMBS'16 Symposium in Khujand will provide a good chance for the opening of the trilateral communication in science between Tajikistan, Japan and Russia.

So far, in September 2016 the delegation of world leading scientists from Russia, Japan and other countries make a first visit to Khujand, Tajikistan' north capital and held a new international symposium KSCMBS-2016, hosted by Khujand state University named after Academician B. Gafurov of the Ministry of Education and Science of the Republic of Tajikistan. The Organizing committee was as: Anvar Maqsudi - Rector of HGU, Tajikistan; Kholmurzo T. Kholmurodov - Co-Chairman from JINR, Dubna, Moscow region, Russia; Kenji Yasuoka - Co-Chairman from Keio University, Japan; Roman G. Efemov - Co-Chairman from IBCh, Russian Academy of Sciences, Moscow, Russia; Tomoyuki Yamamoto - Co-Chairman from Waseda University, Japan; Yuko Okamoto - Co-Chairman from Nagoya University, Japan.

The KSCMBS-2016 symposium has appeared to provide an ideal opportunity to discuss the latest development and exchange technical ideas in the field of computational materials and biological sciences. This symposium is a 2nd international symposium held in Tajikistan following the 1st one held in Dushanbe in 2014. Especially, as organizers were planning, the KSCMBS-2016 would promote to establish the very close cooperation between young researchers that help to strengthen the future scientific cooperation between Tajikistan, Russia and Japan. In the framework of the KSCMBS the presentation talks and lectures would be given not only by leading Russian and Japanese scientists, but also by young researchers from

Russia and Japan covering the following topics: the development of high performance computers and new theoretical methods; computational methods in modern materials and biological sciences, and so on. The contributions of Tajikistani scientists are greatly welcome to make their bridges with Japanese and Russian colleagues and to promote a new branch of world science in the own country.

In particular, the research topics that covered at KSCMBS-2016 were as follows:

- Computer molecular simulation methods and approaches
- Molecular dynamics (MD) and Monte-Carlo (MC) techniques
- Modeling of biological molecules (RNA, DNA, proteins, enzymes, mutation transitions, etc.)
- Physical and biochemical systems (gasses, crystals, liquids, polymers, bio-tribology, etc.)
- Material fabrication and design (ion doped structures, high pressure clathrates, carbon nanotubes)
- Drug design in medicine (docking of one molecule to another, inhibitory activities of enzymes)
- Computational and computing physics, chemistry, biology and medicine
- GPU accelerated molecular dynamics & related techniques

The representatives of the research institute and universities that participated the KSCMBS-2016 symposium included: Keio, Waseda, Nagoya and Kyoto Universities (Japan), Joint Institute for Nuclear Research (Russia, Dubna), Lomonosov Moscow State University (Russian Federation), Joint Institute for High Temperatures (RAS, Moscow), Institute of Bioorganic Chemistry (RAS, Moscow), Groningen University (The Netherlands), JNU (India), so on.

Such high level Japan-Russia-Tajikistan conferences with active contributions of scientists from Europe, USA and other countries are focused on the computational simulation, mainly on the molecular dynamics simulation, thereby serving as an example of rapid informational and technological exchanges in our rather fast changing world of creation of new materials, new drugs and new scientific-educational tools. It is also important to note the cultural and humanitarian exchanges between the delegations of the participating countries on the KSCMBS-2016 International Symposium.

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Organizing Chairman

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