Project Title:

MD Simulations on Si-Clathrates and Biomolecules with DL_POLY/MDGRAPE-3 and AMBER

Name:

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1. Since 1997, our research teams from JINR (Principal: Dr. Kholmirzo KHOLMURODOV) and RIKEN (Principal: Dr. Toshikazu EBISUZAKI) have been performing long-term and very productive joint research on molecular dynamics simulation of material science and biological problems. We have published several joint papers in international and domestic scientific journals; presented joint papers at international meetings and conferences. We have organized and successfully performed several International Workshops "Molecular Simulation Studied in Material and Biological Sciences" (MSSMBS) in 2004, 2006, 2008, and 2010 on methodological and application aspects of the art of molecular dynamics simulation. We have experience of joint MD research on different kinds of computers of parallel or vector architectures. During many years, we have been developing simulation techniques, methods, and computer codes under specialized computing architectures, like MDGRAPE-2 and 3 (Tflop and Pflop calculation speed for large biological systems).
2. Quick Use Status of the RICC System. Molecular Dynamics (MD) Calculation Method.
3. New Structural Data on Si-Clathrates At High Pressures. Novel Protein Strucutral and Functional Properties at Physiological Temperatures.
4. The Use of the MD Simulation Method is One of the Effective Approach for Discovering New Phenomena and Structural Properties of the Nano-Bio-System.
5. April 2011 – April 2012.
6. We continue MD simulations for the several system sizes on the objects as outlined in the project. The obtained simulation data indicate on the possible pathways of the dynamical changes and structural behavior.

Fiscal Year 2010 List of Publications Resulting from the Use of RICC

[Publication]

1. Kholmirzo Kholmurodov, Evgenii Krasavin, Viktor Krylov, Ermuhammad Dushanov, Vladimir Korenkov, Kenji Yasuoka, Tetsu Narumi, Yousuke Ohno, Makoto Taiji, Toshikazu Ebisuzaki, "Molecular Dynamics Studies on the Structure of Onco-Proteins P53: Correlation Between the Wild-Type and Radioresistant Mutant Systems", In: Book of Abstracts of the 4th JAPAN – RUSSIA INTERNATIONAL WORKSHOP MSSMBS'10 "Molecular Simulation Studies in Material and Biological Sciences", JINR-MSU, Dubna-Moscow, September 26 – 29, 2010. ISBN 978-5-9530-0256-1, Kholmurodov Kh.T. (Editor).
2. Kholmirzo Kholmurodov, Alena Chulkova, Kenji Yasuoka, "Molecular Dynamics Study of the Effect of Electrostatic Interactions on the Biphenyl Structure in the Active HNO3 Solvent", The Open Physical Chemistry Journal, 2010, 4, pp. 10-16, ISSN: 1874-0677 http://www.bentham.org/open/topcj/openaccess2.htm
3. Kholmirzo Kholmurodov, Guzel Aru, Kenji Yasuoka, "Molecular dynamics simulations of the interaction of carbon nanotube and a carbon disulfide solvent", Natural Science, 2010, Vol.2, No.8, pp.902-910. http://www.scirp.org/journal/ns/
4. Kholmirzo Kholmurodov, Maria Abasheva, Kenji Yasuoka, "Molecular dynamics simulations of valinomycin interactions with potassium and sodium ions in water solvent", Advances in Bioscience and Biotechnology, 2010, Volume 1, Number 3, pp. 145-240, ISSN Print: 2156-8456
5. E. Dushanov, Kh. Kholmurodov, G. Aru, V. Korenkov, W. Smith, Y. Ohno, T. Narumi, G. Morimoto, M. Taiji, K. Yasuoka, "MD simulations with different computing cluster and communication architectures" // Physics of Particles and Nuclei Letters, 2009, Vol. 6, No. 3, pp. 251-256.

[Proceedings, etc.]

1. Kholmurodov Kh.T. (Editor) 4th JAPAN-RUSSIA INTERNATIONAL WORKSHOP "MOLECULAR SIMULATION STUDIES IN MATERIAL AND BIOLOGICAL SCIENCES", Nova Science Publishers (N.Y.), ISBN: , 2011 (in press).

[Oral presentation at an international symposium]

4th JAPAN-RUSSIA INTERNATIONAL WORKSHOP "MOLECULAR SIMULATION STUDIES IN MATERIAL AND BIOLOGICAL SCIENCES", JINR-MSU, Dubna-Moscow, September 26 – 29, 2010.

[Others]