Project Title:

MD Simulations on Material Science Models and Biomolecules

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1. Background and purpose of the project, relationship of the project with other projects

We have performed molecular dynamics (MD) simulations for materials science and biological subjects. We do have experiences 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). We published joint papers in international and domestic scientific journals; presented joint studies at international meetings and conferences. We have organized and successfully performed several Japan-Russia International Workshops "Molecular Simulation Studied in Material and Biological Sciences" (MSSMBS) in 2004-2012, The MSSMBS workshops are devoted to methodological and application aspects of the art of molecular dynamics simulation.

2. Specific usage status of the system and calculation method

General Use Status of the RICC System. Molecular Dynamics (MD) Calculation Method.

3. Result

New Structural Data of Nano- and Biomolecules.

4. Conclusion

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. Schedule and prospect for the future

April 2012 – April 2013.

6. If you wish to extend your account, provide usage situation (how far you have achieved, what calculation you have completed and what is yet to be done) and what you will do specifically in the next usage term.

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 2012 List of Publications Resulting from the Use of RICC

[Publication]

1. Kholmirzo Kholmurodov, "Molecular Dynamics Study of the Effect of Induced Mutations on the Protein Structures Associated with Diseases of A Radiobiological Nature" American Journal of Bioscience and Bioengineering, 2013, 1(1), 7-16. DOI: 10.11648/j.bio.20130101.12
2. Dushanov E., Kholmurodov Kh., Yasuoka K., Krasavin E., "MD Studies on Conformational Behavior of a DNA Photolyase Enzyme", PEPAN Letters, 2013, 10 (6) (in press).
3. Kholmirzo Kholmurodov, Ermuhammad Dushanov, Kenji Yasuoka, Hagar Hassan, Ahmed Galal, Nasser Sweilam, "Structural and Diffusional Study of Pure Ethanol and Water on Pt(III) Surface Using Molecular Dynamics Simulation" Eur. Chem. Bull. 2013, 2(5), 247-254
4. R.A. Eremin, Kh.T. Kholmurodov, V.I. Petrenko, M.V. Avdeev, "Calculating the Bulk Properties of Decalines and Fatty Acids Decaline According to Data from Molecular Dynamics Simulation", Russian Journal of Physical Chemistry A, 2013, Vol. 87, No. 5, pp. 745-751. © Pleiades Publishing, Ltd., ISSN 0036 0244, 2013.
5. Roman EREMIN, Kholmirzo KHOLMURODOV, Viktor PETRENKO, László ROSTA and Mikhail AVDEEV, "The effect of the solute-solvent interface on the small-angle neutron scattering from organic solutions of short alkyl chain molecules as revealed by molecular dynamics simulation" Journal of Applied Crystallography, Volume 46, Part 2 (April 2013) doi:10.1107/S002188981205131X
6. Kholmirzo T. Kholmurodov, Ermuhammad B. Dushanov, Evgenii A. Krasavin, Hagar K. Hassan, Hadeer A. ElHabashy, Ahmed Galal, Nasser H. Sweilam, and Kenji Yasuoka, "Molecular Dynamics Simulations of the DNA Interaction with Metallic Nanoparticles and TiO_2 Surfaces", JINR Preprint, E19-2013-17, Dubna, 2013. (in press)
7. Dushanov E.B., Kholmurodov Kh.T., Yasuoka K., and Krasavin E.A., "A Comparative MD Analysis of the Structural and Diffusion Properties of Formamide/Water and Ethanol/Water Mixtures on TiO_2 and Pt Surfaces", JINR Preprint, E17-2013-18, Dubna, 2013. (in press)
8. Kholmurodov Kh.T., "ON THE CORRELATION EFFECTS BETWEEN THE MOLECULAR MECHANISMS OF PROTEIN STRUCTURE CHANGES AND DISEASES OF A RADIOBIOLOGICAL NATURE", Book of abstracts, 2nd Biotechnology World Congress 2013, February 18th - 21st, 2013 Dubai, UAE
9. Ermuhammad DUSHANOV, Kholmirzo KHOLMURODOV and Kenji YASUOKA, "Activation energy calculations for formamide-TiO2 and formamide-Pt interactions in the presence of water" The Open Biochemistry Journal, (in press),
10. Roman EREMIN, Kholmirzo KHOLMURODOV, Viktor PETRENKO, László ROSTA and Mikhail AVDEEV, "SANS data modeling based on MD simulation: saturated mono-carboxylic acids solutions", Proceedings of SNCSR-2012, October 15-19, 2012, St. Petersburg, Russia.
11. Kholmirzo KHOLMURODOV (Editor), 5th JAPAN-RUSSIA International Workshop "Molecular Simulation Studies in Material and Biological Sciences" (MSSMBS2012), September 09-12, 2012, JINR-IBC RAS, Dubna-Moscow, Book of Abstracts,
    ISBN 978-5-9530-0336-0, E19-2012-90.
12. Kholmirzo KHOLMURODOV, "Molecular Modeling in Biological (Protein) and Material Research", Scientific Seminar of Thermal Physics Laboratory,
    Department of Engineering Physics and Mechanics, Graduate School of Engineering, 20 July 2012, KYOTO UNIVERSITY, Japan.
13. Kholmirzo KHOLMURODOV, "Molecular Dynamics Simulations of Nano- and Biostructures", Scientific Seminar of Yasuoka Laboratory, Department of Mechanical Engineering, Faculty of Science and Technology, 24 July 2012, KEIO UNIVERSITY, Japan.
    Tatyana FELDMAN, Mikhail OSTROVSKY, Kholmirzo KHOLMURODOV, and Kenji YASUOKA, "Model of Abnormal Chromophore-Protein Interaction for E181K Rhodopsin Mutation: Computer Molecular Dynamics Study", The Open Biochemistry Journal, 6, 94-102, 2012; DOI: 10.2174/1874091X01206010094, ISSN: 1874-091X.
    http://www.ncbi.nlm.nih.gov/pmc/journals/678/.
14. Kholmirzo Kholmurodov, "Computer Molecular Simulation of Nano- and Biostructures", Scientific Seminar of Laboratory for Computational Molecular Design, Computational Biology Research Core, Quantitative Biology Center (QBiC), 11 July 2012, RIKEN, Kobe, Japan.
15. Kholmirzo Kholmurodov, Ermuhammad Dushanov, Kenji Yasuoka, "Molecular Dynamics Simulations of a DNA Photolyase Protein : High-Mobility and Conformational Changes of the FAD Molecule at Low Temperatures", Advances in Bioscience and Biotechnology, Vol.3 No.3, June 2012, PP.169-180, DOI: 10.4236/abb.2012.33025.
16. Roman Eremin, Kholmirzo Kholmurodov, Mikhail Avdeev, Viktor Petrenko, László Rosta, "Molecular dynamics simulation in modeling of SANS: solutions of mono-carboxylic acids in decalin" 6th Central European Training School on Neutron Scattering (14 May - 19 May, 2012, Budapest, Hungary)

17. Roman Eremin, Kholmirzo Kholmurodov, Viktor Petrenko, Mikhail Avdeev, "Molecular dynamics simulations on pure *cis-* and *trans-*decalin solutions and their mixtures" XVI Conference of Young Scientists and Specialists (AYSS'12), 06 - 11 February, 2012, JINR, Dubna, Russia
18. Kholmirzo Kholmurodov, Ermuhammad Dushanov, Roman Eremin, Donguk Suh, Kenji Yasuoka, "Molecular Dynamics Simulations of Vapor Heterogeneous Nucleation on a Graphite Surface", XVIth Research Workshop Nucleation Theory and Applications, Dubna, Russia April 1 - 30, 2012
19. Roman Eremin, Kholmirzo Kholmurodov, Mikhail Avdeev, Viktor Petrenko, Kenji Yasuoka, "Molecular Dynamics Simulation on *trans-* and *cis-*Decalins: The Effect of Partial Atomic Charges and Adjustment of "Real Densities"", International Journal of Chemistry, Canadian Center of Science and Education, Vol.4, No.1; pp.14-23 (2012)
20. Kholmirzo Kholmurodov, Ermuhammad Dushanov, Kenji Yasuoka, Hagar Khalil, Ahmed Galal, Sameh Ahmed, Nasser Sweilam, Hatem Moharram, "Molecular dynamics study of ethanol solvated by water on a Pt(111) surface", CHEMICAL PHYSCIS, Volume 402, 19 June 2012, Pages 41-47, http://dx.doi.org/10.1016/j.chemphys.2012.04.002
21. E. Dushanov, Kh. Kholmurodov, and K. Yasuoka, "Molecular dynamics studies of the interaction between water and oxide surfaces", PEPAN Letters, 2012, v.9, 5(175), pp. 876-891
22. E. Dushanov, Kh. Kholmurodov, and K. Yasuoka, "The diffusion and concentration effects of formamide on a TiO2 surface in the presence of a water solvent", Natural Science, Vol.4 No.5, May 2012, DOI: 10.4236/ns.2012.45044
23. Kholmirzo Kholmurodov, "On the Correlation Effects Between the Molecular Mechanisms of Protein Structure Changes and Diseases of a Radiobiological Nature", International Seminar on Radioactivity, Curies and Social Commitments of the Scientists, Invited Talk at The Asiatic Society, Kolkata, India.
24. Kholmirzo Kholmurodov, Ermuhammad Dushanov, Kenji Yasuoka, Hagar Khalil, Ahmed Galal, Sameh Ahmed, Nasser Sweilam, Hatem Moharram, "Molecular Dynamics Simulation of the Interaction of Ethanol-Water Mixture with a Pt Surface", Natural Science, Vol.3 No.12, December 2011, DOI: 10.4236/ns.2011.312126
25. Kholmirzo Kholmurodov, Ermuhammad Dushanov, Kenji Yasuoka, "MD Simulations of the P53 oncoprotein structure: the effect of the Arg273 → His mutation on the DNA binding domain", Advances in Bioscience and Biotechnology, Volume 2, Number 5, October 2011, DOI: 10.4236/abb.2011.25048
26. Kholmurodov Kh.T. (Editor) MOLECULAR DYNAMICS OF NANOBIOSTRUCTURES, Nova Science Publishers (New York), ISBN: 978-1-61324-320-6, 2011, 150 pages.
27. "Homology Modelling and Molecular Dynamics of Cyclin-Dependent Protein Kinases" by Robert A. Selwyne, Kholmirzo T. Kholmurodov, Natalia A. Koltovaya, has been published by IT for Real Rorld Problems, (Universities Press Series in Systems, Models, Informatics and Control), Ed. Sree Hari Rao (Ed.), pp. 1-72.
28. Kh.T. Kholmurodov, E.A. Krasavin, V.A. Krylov, E.B. Dushanov, V.V. Korenkov, K. Yasuoka, T. Narumi, Y. Ohno, M. Taiji, T. Ebisuzaki, "MD Simulations on the Structure of Onco-Proteins P53: Wild-Type and Radioresistant Mutant Systems", In: "MOLECULAR DYNAMICS OF NANOBIOSTRUCTURES", Nova Science Publishers (N.Y.), ISBN: 978-1-61324-320-6, 2012.
29. Kh.T. Kholmurodov, T.B. Feldman, M.A. Ostrovsky, "Chromophore Rearrangement in Binding Pocket of Rhodopsin Makes Sense for its Physiological Dark-Adapted State: Computer Molecular Simulation Study" In: "MOLECULAR DYNAMICS OF NANOBIOSTRUCTURES", Nova Science Publishers (N.Y.), ISBN: 978-1-61324-320-6, 2012.

[Proceedings, etc.]

1. Kholmurodov Kh.T. (Editor). “Models in Bioscience and Materials Research: Molecular Dynamics and Related Approach”, Proceedings of 5th JAPAN-RUSSIA INTERNATIONAL WORKSHOP “MOLECULAR SIMULATION STUDIES IN MATERIAL AND BIOLOGICAL SCIENCES”, Nova Science Publishers (N.Y.), 159 pages, 2013 (in press).

[Oral presentation at an international symposium]

5th JAPAN-RUSSIA INTERNATIONAL WORKSHOP “MOLECULAR SIMULATION STUDIES IN MATERIAL AND BIOLOGICAL SCIENCES”, JINR-IBC, Dubna-Moscow, September 09 – 12, 2012.