Project Title:

MD Simulations on Material Science Models and Biomolecules

Name: ○Kholmirzo Kholmurodov, Toshikazu Ebisuzaki, Toshiaki Iitaka

Laboratory at RIKEN: Computational Astrophysics Laboratory

1. Molecular dynamics (MD) simulations for materials science and biological subjects. Joint papers in international and domestic scientific journals; presented joint studies at international meetings and conferences as Japan-Russia International Workshops "Molecular Simulation Studied in Material and Biological Sciences" (MSSMBS) in 2004-2012.
2. General Use Status of the RICC System. Molecular Dynamics (MD) Calculation Method.
3. New Structural Data of Nano- and Biomolecules.
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 2012 – April 2013.
6. I wish to extend my account.

Fiscal Year 2013 List of Publications Resulting from the Use of RICC

[Publication]

Books; Chapters in books

1. Kholmirzo KHOLMURODOV (Editor), "Models in Bioscience and Materials Research: Molecular Dynamics and Related Techniques", Nova Science Publishers (N.Y.), 2013.

Papers [2013]

2. Kholmirzo Kholmurodov, "MD Studies on the Structures of the DNA Photolyase Enzyme and Visual Pigment Rhodopsin", Abstracts of the 1st ISCMBS, "International Symposium on Computational Materials & Biological Sciences", Waseda University, Tokyo, Japan, 10-12 September, 2013.
3. R. Eremin, Kh. Kholmurodov, V. Petrenko, M. Avdeev, L. Rosta, "Monocarboxylic acids organic solutions: Solute solvent interface area effect on the SANS data as revealed by MD", Abstracts of the 1st ISCMBS, "International Symposium on Computational Materials & Biological Sciences", Waseda University, Tokyo, Japan, 10-12 September, 2013.
4. Tatyana Feldman, Mikhail Ostrovsky, Kholmirzo Kholmurodov, "Studies on retinal chromophore functions of visual pigment rhodopsin in normal and pathology versions", Abstracts of the 1st ISCMBS, "International Symposium on Computational Materials & Biological Sciences", Waseda University, Tokyo, Japan, 10-12 September, 2013.
5. Еремин Р.А., Холмуродов Х.Т., Петренко В.И., Rosta L., Авдеев М.В., "Анализ малоуглового рассеяния нейтронов раствором стеариновой кислоты в бензоле с использованием молекулярно-динамического моделирования" Физика твердого тела, Принята в печать 2014, том 56, выпуск 1.
6. E. Dushanov, Kh. Kholmurodov and K. Yasuoka, "Structural and Diffusion Properties of Formamide/Water Mixture Interacting with TiO2 Surface" Bioorganic Chemistry, 2013, 50, pp. 11-16. [DOI: 10.1016/j.bioorg.2013.07.002]
7. Kholmirzo KHOLMURODOV (Editor), "Models in Bioscience and Materials Research: Molecular Dynamics and Related Techniques", Nova Science Publishers (N.Y.), Proceedings of the 5th JAPAN-RUSSIA International Workshop "Molecular Simulation Studies in Material and Biological Sciences" (MSSMBS'12), JINR-IBC RAS, Dubna-Moscow, September 09-12, 2012, 159 pages (in press).
8. 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, 2013, 7, pp. 33-43, [DOI: 10.2174/1874091X01307010033].
9. 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].
10. Dushanov E., Kholmurodov Kh., Yasuoka K., Krasavin E., "MD Studies on Conformational Behavior of a DNA Photolyase Enzyme", PEPAN Letters, 2013, 10 (6), pp. 974-985.
11. (Душанов Э., Холмуродов Х., Ясуока К., Красавин Е., "МД исследования конформационного поведения фермента ДНК-фотолиазы", Письма в ЭЧАЯ, 2013, 10 (6), стр. 974-985.)
12. 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
13. Р.А. Еремин, Х.Т. Холмуродов, В.И. Петренко, М.В. Авдеев, "Расчет объемных свойств декалинов и жирных кислот в декалине по данным молекулярно-динамического моделирования", Журнал физической химии, 2013, 87 (5), 759-765.
14. (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. [DOI: 10.1134/S0036024413040092])

15. 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].
16. Халанский Д.А., Холмуродов Х.Т., Душанов Э.Б., Гладышев П.П., "Модели жидких элекролитов на основе молекулярной динамики" Материалы научного семинара, посвященного научной деятельности профессора И.Л. Ходаковского, с. 175-180, Международный университет природы, общества и человека, "Дубна", [ISBN 978-5-89847-378-5].
17. 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 TiO2 Surfaces", JINR Preprint, E19-2013-17, Dubna, 2013.
18. 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 TiO2 and Pt Surfaces", JINR Preprint, E17-2013-18, Dubna, 2013.
19. 16.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
20. 17.Р.А. Еремин, Х.Т. Холмуродов, В.И. Петренко, М.В. Авдеев, Л. Рошта, "Приложение метода МД моделирования к анализу данных МУРН разбавленными растворами монокарбоновых кислот" Тезисы докладов, с. 111, 2013. 47-ая Школа ПИЯФ по физике конденсированного состояния (ФКС-2013), ФГБУ ПИЯФ им. Б.П. Константинова, Зеленогорск, Россия, 2013
21. 18.Р.А. Еремин, Х.Т. Холмуродов, В.И. Петренко, М.В. Авдеев, "МОЛЕКУЛЯРНО-ДИНАМИЧЕСКОЕ МОДЕЛИРОВАНИЕ ВЗАИМОДЕЙСТВИЯ РАСТВОРИТЕЛЬ-РАСТВОРЕННОЕ ВЕЩЕСТВО В НЕПОЛЯРНЫХ РАСТВОРАХ ОЛЕИНОВОЙ КИСЛОТЫ", Поверхность. Рентгеновские, синхротронные и нейтронные исследования, 2013 (в печати)
22. (R.A. Eremin, Kh.T. Kholmurodov, V.I. Petrenko, M.V. Avdeev, "SOLUTE-SOLVENT INTERACTION IN NONPOLAR SOLUTIONS OF OLEIC ACID AS REVEALED BY MOLECULAR DYNAMICS SIMULATION", The Journal of Surface Investigation. X-ray, Synchrotron and Neutron Techniques, 2013 (in press)
23. 19.Kholmirzo Kholmurodov, Ermuhammad Dushanov, Roman Eremin, Donguk Suh, Kenji Yasuoka, "On Heterogeneous Water Vapor Nucleation inside Carbon Nanopores". 17th Research Workshop Nucleation Theory and Applications (NTA-2013), JINR, Dubna, Russia, April 1 - 30, 2013
24. 20.Ermuhammad Dushanov, Kholmirzo Kholmurodov, Kenji Yasuoka and Evgenii Krasavin, "Chapter 2. MD Studies of the Structural and Diffusion Properties of Formamide/Water and Ethanol/Water Mixtures on Titanium and Platinum Surfaces". In: Models in Bioscience and Materials Research: Molecular Dynamics and Related Techniques, Editor: Kholmirzo T. Kholmurodov, Nova Science Publishers Ltd. (New York), 2013 [ISBN: 978-1-62808-052-0]
25. 21.Roman A. Eremin, Kholmirzo T. Kholmurodov, Viktor I. Petrenko, Laszlo Rosta and Mikhail V. Avdeev, "Chapter 10. Molecular Dynamics Simulations for Small-Angle Neutron Scattering: Scattering Length Density Spatial Distributions for Mono-Carboxylic Acids in d-Decalin". In: Models in Bioscience and Materials Research: Molecular Dynamics and Related Techniques, Editor: Kholmirzo T. Kholmurodov, Nova Science Publishers Ltd. (New York), 2013 [ISBN: 978-1-62808-052-0]
26. 22.Kholmirzo T. Kholmurodov, Ermuhammad B. Dushanov, Evgenii A. Krasavin, Hagar K. Hassan, Hadeer A. ElHabashy, Ahmed Galal, Nasser H. Sweilam and Kenji Yasuoka, "Chapter 12. Molecular Dynamics Simulations of the DNA Interaction with Metallic Nanoparticles and TiO2 Surfaces". In: Models in Bioscience and Materials Research: Molecular Dynamics and Related Techniques, Editor: Kholmirzo T. Kholmurodov, Nova Science Publishers Ltd. (New York), 2013 [ISBN: 978-1-62808-052-0]
27. 23.Халанский Д.А., Холмуродов Х.Т., Душанов Э.Б., Гладышев П.П., "Жидкостные

модели элекролитов на основе молекулярной динамики", Тезисы докладов 3-ей научной конференции с международным участием «Химия-2013. Физическая химия. Аналитическая химия. Нанохимия. Теория, эксперимент, практика, преподавание» (Московский областной университет, научно-образовательный центр "Биология клетки и биотехнология", 14-16 марта 2013 г.): стр. 102, сб. тезисов докладов/коллектив авторов. - М.:Изд-во МГОУ, 2013. - 120 с. [УДК 54:37.016(043) ББК 74.262.4].

28. 24.Kholmurodov Kh.T., Dushanov E.B., Yasuoka K., Krasavin E.A., "A comparative MD analysis of formamide/water and ethanol/water mixtures on TiO2 and Pt surfaces". International Conference of Actual Problems of Molecular Spectroscopy of Condensed Matter, Samarkand, 2013, May 29-31, Book of abstracts, pp. 59-60 [ISBN: 978-9943-4193-0-8]
29. 25.Dushanov E.B., Kholmurodov Kh.T., Yasuoka K., Krasavin E.A., "Low temperature conformational dynamics of a FAD molecule and a DNA photolyase protein". International Conference of Actual Problems of Molecular Spectroscopy of Condensed Matter, Samarkand, 2013, May 29-31, Book of abstracts, pp. 60-61 [ISBN: 978-9943-4193-0-8]
30. 26.Kholmurodov Kh.T., "Molecular dynamics studies of the DNA photolyase enzyme and visual pigment rhodopsin: specifics of the chromophore conformations". International Workshop Computational and theoretical modeling of biomolecular interactions, July 3-8, 2013, Dubna, Russia, Book of abstracts, pp. 26-29 [ISBN: 978-5-4344-0126-5] Presentation
31. 27.Артошина О.В., Воробьева М.Ю., Душанов Э.Б., Холмуродов Х.Т., "Молекулярно-динамическое моделирование процессов взаимодействия формамида с синильной кислотой в присутствии катализатора TiO2", Препринт ОИЯИ, Р18-2013-64, Дубна, 2013.(в печати, направлено в "Журнал физической химии")
32. 28.Артошина О.В., Воробьева М.Ю., Душанов Э.Б., Холмуродов Х.Т., "Молекулярно-динамическое моделирование процессов взаимодействия формамида с синильной кислотой в присутствии катализатора TiO2", Журнал физической химии, 2013.(в печати)
33. (Artoshina O.V., Vorobeva M.Yu, Dushanov E.B., Kholmurodov Kh.T., "Molecular Dynamics Simulations of the Formamide Interaction with Hydrocyanic Acid on a Catalytic Surface TiO2", Russian Journal of Physical Chemistry A, 2013.(in press))
34. 29.Kholmurodov Kh, Dushanov E, Yasuoka K, and Krasavin E., "Molecular dynamics studies of chromophores conformational behavior of the visual pigment rhodopsin and DNA photolyase enzyme", Proceedings of The International Conference on Condensed Matter Physics, devoted to 85-th Anniversary of Academician A.A. Adhamov, Tajikistan, Dushanbe, 17-18 October 2013, izd. Donish, p. 51.

[Proceedings, etc.]

1. 1st ISCMBS, "International Symposium on Computational Materials & Biological Sciences", Waseda University, Tokyo, Japan, 10-12 September, 2013.

[Oral presentation at an international symposium]

1. 1st ISCMBS, "International Symposium on Computational Materials & Biological Sciences", Waseda University, Tokyo, Japan, 10-12 September, 2013.

[Others]