Program

1st International Symposium on Computational Materials and Biological Sciences

Sep. 10-12, Waseda University, Tokyo, Japan

Tuesday, Sep. 10	
17:00-19:00	Registration & Welcome reception

Wednesday, Sep. 11	
8:30-	Registration
9:00-9:10	Welcome: T. Yamamoto (*Waseda Univ.*)
Session I (Chair: K. Kholmurodov, *Joint Institute for Nuclear Research*)	
9:10-9:50 **Invited**	R. Efremov (*Institute of Bioorganic Chemistry*) Dynamic STRUCTURAL/AMPHIPHILIC "PORTRAIT" of biomembranes as their Fundamental property relevant to function: Results of Atomistic Simulations
9:50-10:30 **Invited**	Y. Okamoto (*Nagoya Univ.*) Generalized-ensemble simulations of spin and biological systems
10:30-11:00	Coffee
Session II (Chair: I. Kovalenko, *Lomonosov Moscow State Univ.*)	
11:00-11:20	D. Ustinin (*Lomonosov Moscow State Univ.*) GPU-accelerated Brownian dynamics simulation of protein-protein interactions
11:20-11:40	Y. Inaba (*Waseda Univ.*) Electronic structure of $RE_{1-x}AE_xMnO_{3-\delta}$ (RE = Rare-earth, AE = Alkaline-earth)
11:40-12:00	A. Diakonova (*Lomonosov Moscow State Univ.*) Direct computer simulation of interactions of ferredoxin with its protein partners
12:00-12:20	Y. Oka (*Waseda Univ.*) Driving mechanisms for structural transitions of Ar_7 clusters
12:20-13:30	Lunch
Session III (Chair: T. Akimoto, *Keio Univ.*)	
13:30-14:10 **Invited**	K. Hirose (*JAXA*) Atomic structures and physical properties at ultrathin-SiO_2/Si interfaces
14:10-14:50 **Invited**	I. Kovalenko (*Lomonosov Moscow State Univ.*) Computer simulation of protein-protein interactions
14:50-15:30 **Invited**	H. Matsubara (*Tohoku Univ.*) Physics of nanoconfined liquids: insights from molecular dynamics simulation
15:30-16:00	Poster preview (Chair: S. Ohmura, *Kyoto Univ.*)
16:00-17:20	Poster
17:30-19:30	Banquet

Thursday, Sep. 12	
Session IV (Chair: R. Efremov, *Institute of Bioorganic Chemistry*)	
9:00-9:40 **Invited**	K. Kholmurodov (*Joint Institute for Nuclear Research*) MD studies on the structures of the DNA photolyase enzyme and visual pigment rhodopsin
9:40-10:20 **Invited**	Y. Hirano (*RIKEN*) Computational study of protein-ligand interactions
10:20-10:50	Coffee
Session V (Chair: G. Riznichenko, *Lomonosov Moscow State Univ.*)	
10:50-11:10	A. Chugunov (*Institute of Bioorganic Chemistry*) "Protein surface topography": a novel approach to structure–function studies for bioactive peptides
11:10-11:30	R. Urano (*Nagoya Univ.*) Replica-exchange simulations for structure predictions of alpha-helical membrane proteins
11:30-11:50	T. Feldman (*Joint Institute for Nuclear Research*) Studies on retinal chromophore functions of visual pigment rhodopsin in normal and pathology versions
11:50-12:10	E. Yamamoto (*Keio Univ.*) Water transportation in Aquaporin-1 follows non-Poisson statics
12:10-13:30	Lunch
Session VI (Chair: H. Matsubara, *Tohoku Univ.*)	
13:30-14:10 **Invited**	T. Yanao (*Waseda Univ.*) Geometric effects in shape dynamics of complex molecular systems
14:10-14:50 **Invited**	G. Riznichenko (*Lomonosov Moscow State Univ.*) Simulation of electron and proton transport processes in photosinthetic membrane
14:50-15:30 **Invited**	T. Akimoto (*Keio Univ.*) Aging but equilibrium in water dynamics near the surface of membrane
15:30-16:00	Coffee
Session VII (Chair: T. Yanao, *Waseda Univ.*)	
16:00-16:40 **Invited**	S. Ohmura (*Kyoto Univ.*) Dissociation mechanism of highly charged molecules: *Ab initio* molecular-dynamics simulations
16:40-17:00	R. Eremin (*Joint Institute for Nuclear Research*) Monocarboxylic acids organic solutions: Solute solvent interface area effect on the SANS data as revealed by MD
17:00-17:20	M. Hiratsuka (*Keio Univ.*) Molecular motion analysis of amyl-alcohol in structure II and H clathrate hydrates by molecular dynamics simulation
17:20-17:40	P. Mamonov (*Lomonosov Moscow State Univ.*) An efficient approach to modeling of electron-conformational interactions: the study of self exchange reaction between iron II/III ions in solution
17:40-18:00	Closing: K. Yasuoka

Posters (Sep. 11th, 16:00-17:20)

	Presenter	Title
P1	D. Takaiwa (*Keio Univ.*)	Molecular dynamics simulation of the interaction of nucleotide with a phospholipid bilayer
P2	K. Mori (*Waseda Univ.*)	Substitution mechanism of Mn ions in $CaTiO_3$
P3	Donguk Suh (*Keio Univ.*)	Molecular dynamics simulation of heterogeneous nucleation on various seed shapes
P4	T. Mariya (*Waseda Univ.*)	Local environment analysis of transition metal ions in hexagonal $BaTiO_3$
P5	T. Shibuya (*Keio Univ.*)	DFT study of the bipolaron formation due to oxygen vacancy on (110) TiO_2 surface
P6	S. Yoshioka (*Waseda Univ.*)	Lagrangian coherent structures mediating phase-space flows in unimolecular reactions
P7	K. Tomobe (*Keio Univ.*)	The behavior of conserved water molecules of PrPc and pathogenic mutation T188R by molecular dynamics simulations
P8	T. Oomori (*Waseda Univ.*)	Co K-edge X-ray absorption near-edge structure analysis of Co-doped CeO_2
P9	T. Nozawa (*Keio Univ.*)	Molecular dynamics simulation of 5CB with GPU accelerated Coulombic calculation
P10	K. Meguro (*Waseda Univ.*)	Influence of Eu incorporation on the geometrical structure of Sr_2SnO_4
P11	D. Yuhara (*Keio Univ.*)	Analysis of methane hydrate growth rate by molecular dynamics simulation
P12	S. Wakao (*Waseda Univ.*)	Correlation between breakdown electric-field strength and recovery rate obtained by molecular orbital calculation
P13	K. Nomura (*Keio Univ.*)	Acceleration of replica exchange molecular dynamics simulation on graphics processing units
P14	N. Nishikawa (*Nagoya Univ.*)	Molecular dynamics simulations for understanding the initial process of amyloid formations
P15	N. Yamato (*Keio Univ.*)	Connection of atomistic and coarse-grained molecular simulation of polymer melts based on the Rouse parameters
P16	S. Ito (*Nagoya Univ.*)	Free energy calculation for proton transfer in malonaldehyde using DFTB and REUS
P17	Winarto (*Keio Univ.*)	Study of water-methanol mixture flowing through carbon nanotubes with molecular dynamics simulation