Division of Mathematical and Physical Sciences	Research field	Simulation Science	Lab. ID MP17
Laboratory web site	http://cphys.s.kanazawa-u.ac.jp/home1.html http://cphys.s.kanazawa-u.ac.jp/~oda-web/index.html http://hal.s.kanazawa-u.ac.jp/		

Research subjects

Recent topics on Computational Science in several fields of physics. (1) Computational Solid State Physics: New materials are designed by using parallel computers and supercomputers. We develop methods for simulation based on solid state physics and study electronic structures of metals, semiconductors, carbon nanomaterials, and magnets. We also study molecules and clusters including interstellar ones. (2) Theoretical and Computational Nanoscience: magnetic properties of materials, crystal grouth, surface/interface physics, nanosicence by first principle calculation and first principle molecular dynamics simulation. (3) Computational Biophysics: analysis of functions of proteins and biomolecules such as biological sciences and biophysics by Molecular dynamics simulation and Monte Carlo method in parallel computers and supercomputaers.

Master/Doctor course: Education policy, curriculum, typical activity in the laboratory

Master course students take lectures and join seminars. Conduct research of each research topics and complete master's theses. Doctor students conduct research under supervisors and complete doctoral theses.

Daily life in the laboratory, etc.

PC is assign to each student. Students can use supercomputers in other universities and thus carry out large-scale numerical simulation.

Message or comments by the laboratory faculty staffs

Computational science is the third science in addition to expeimental and theoretical sciences. We hope that students conduct reserch of this new science with special interests.

Recent Master theses in these 3 years (+ more if appropriate)

year.month	Thesis title (including English translation of Japanese thesis title)
2017.9	Development of classical molecular dynamics for magnetic oxygen systems
2017.9	Study of CO adsorption on Ni(111) surface using van der Waals density functional
2017.9	First-principles study on spin-orbit coupling in thin films and interfaces
2017.9	First-principles study on electronic and magnetic structures of nickel cobaltite spinel
2017.3	Theoretical study on self-assembly process and shape deformation of lipid membranes by coarse-grained model
2017.3	First-principles study on the spin-orbit splitting in III-V compound semiconductors
2017.3	Simulation of positron annihilation in crystals
2017.3	Theoretical study on intermolecular interaction and structural stability of protein complex by using the Go-like model
2017.3	Brownian dynamics simulation about control of the two-dimensional structure formed by two components of particles
2017.3	Theoretical study on structural stability of lipid bilayer membrane by membrane potential
2017.3	First-principles study on the electronic structures in Tl/Ag(111) surface and solid oxygen
2017.3	Electronic structure calculations of muoniums in semiconductors
2016.9	First-Principles Calculations of Li-intercalated Bilayer Graphene
2016.9	First-Principles Calculation of Layer Distances in Multi-layer Graphenes
2016.9	Effect of apex angle and deviation of external force direction on crystallization of Brownian particles by sedimentation in the square pyramidal container
2016.9	Theoretical Study of Buckminsterfullerene Formation Pathway from Polycyclic Aromatic Hydrocarbon in Interstellar Medium
2016.3	Control of the structure of colloidal crystals by the shape of pyramidal container and external force
2016.3	Ab initio study on dioxygen coordinated iron porphyrin complex considering hemoglobin environment
2016.3	First-Principles Calculations of Hydrogen Adsorbed in Two-Dimensional Honeycomb Structures

2016.3	Theoretical study of interaction between multilamellar membranes and stability of multilamellar membranes
2016.3	First-principles study on electronic structure and anomalous Rashba effect in Tl-Pb alloy on Si(111) surface
2016.3	Theoretical study on structural dynamics and elasticity of lipid bilayer and mixed membrane
2016.3	Theoretical study on the association-dissociation process of metalloproteins in the photosynthetic reaction
2015.9	First-principles study on electronic structure and magnetic anisotropy variations by electric field in the Fe/oxide-insulator interfaces
2015.9	Prediction of Solvation Free Energy of Proteins and Organic Molecules: Molecular Dynamics Simulation and QSPR Model Approach
2015.9	Electronic Structure Calculations of Hydrogen Impurity in Gallium Nitride
2015.9	First principles calculation of multiferroic BiFeO3 for photovoltaic application
2015.3	Pattern formation by moving particles source-Phase field simulation-
2015.3	Simulation of crystallization of Brownian partilces by Brownian dynamics method
2015.3	Electronic Structure Calculations of Ni substrates
2015.3	Analysis of Electronic Structures of Graphene and Silicene based on Group Theory
2015.3	Theoretical Study on Anomalous Thermoelectric Effets Induced by the Topology of Electronic States
2015.3	Theoretical Quest for Topological Insulators from First-Principles Calculation
2015.3	Theoretical study of structure formation of vesicle arising from interactions between lipids by a coarse-grained model
2014.9	Group Chase and Escape with an Off-lattice Model
2014.9	Pure Rotational Spectroscopy of Neutral and Charged Titanium Oxide Molecules
2014.9	Magnetic Dipole-dipole Interaction Calculation and Magnetic Structure in Solid Oxygen
2014.9	Molecular Dynamics Study of Human Defensins HNP-1 Binds to DPPC Membrane: Structure and Stability
2014.3	Reation between process and requency in cancer-causing
2014.3	Simulation of electronic states of silicene
2014.3	Simulation of PCBM adsorbed on Titanium Oxide
2014.3	Study on an ab initio approach to free-energy reconstruction using logarithmic mean force dynamics
2014.3	Investigating the electronic structure of the polar Zinc Oxide slab based on the first-principles calculation
2014.3	Development and implementation of van der Waals density functional approach
2014.3	First-Principles Study of Spin-Orbit Interaction in Ferroelectrics
2014.3	Development of algorithm for a parallel computing of a excess chemical potential calculation and its application for hydration effect on complex of proteins
2014.3	Theoretical study on structural stability and dynamics of the satellite tobacco mosaic virus by Gō-like model
2014.3	Theoretical studies on a parallel computing for coarse-grained simulation and structure stability of vesicles
2014.3	Theoretical study of dependence of solvent effect of the oxidation-reduction potential on the oxidation of water
2013.9	First—Principles Calculations of Water Molecules Adsorbed on Graphene
2013.9	Implementation of Parallel Matrix Diagonalization for Ab-Initio Molecular Dynamics Program using ScaLAPACK
2013.9	Tight-Binding Molecular Dynamics with Fermi Operator Expansion: Application to Silicon Defects
2013.9	Co Impurity on Fe/MgO Interface: a First Principles Study
2013.9	Computational Study of Oxidation Potential Fluctuation of Ketone Molecule
2013.9	An Approach for Combining Docking and Molecular Dynamics (MD) Simulation In Protein-Ligand Docking
2013.3	First-Principles Calculations of Silicon Vacancies
2013.3	First-principles study on electronic structure and anomalous Rashba effect in Tl/Si(111) surface
2013.3	First-principles study on magnetic anisotropy and its electric field effect in thin films
2013.3	First-Principles Study of Hydrogen-Bonded Dielectrics H2C4O4
2013.3	Theoretical study of structural stability of dihydrofolate reductase by molecular dynamics simulation
2013.3	Theoretical study of bonding between protein and linkages substrate molecule by molecular dynamics simulation
2012.9	First Principles Calculations of Hydrogen Adsorption on Armchair Edge (5,5) Carbon Nanotubes

2012.9	First Principles Calculations of Hydrogen Chemisorption on Zigzag Edge (10,0) Carbon Nanotubes
2012.9	Structural, magnetic and electronic properties in small bismuth clusters
Recent Doctoral theses in these 3 years (+ more if appropriate)	
year.month	Thesis title (including English translation of Japanese thesis title)
2016.9	Development and application of spin dependent van der Waals density functional method
2015.9	Density-functional theory based calculations of spin-orbit interaction in ZnO
2015.9	First-principles calculations of vacancies in semiconductors
2015.3	Theoretical Study of Spin Structures and Physical Properties of Transition Metal Oxides
2015.3	Theoretical Studies on Redox Potential of Molecules by Molecular Dynamics simulation
2014.9	First-Principles Electronic-Structure Calculations of Functional Materials
2014.9	First-Principles Calculations of Polythiophene Derivatives
2014.9	Theoretical studies of the formation mechanism of protein complex by using coarse-grained models
2014.9	Theoretical Studies of the Dependence of Chemical Reaction on Tautomeric Form of His64 in the Active Site of Human Carbonic Anhydrase Ⅱ
2013.9	Study of Carbon Nanomaterials Based on Density Functional Theory
2013.3	Relativistic Electronic State Calculations of Bi ultrathin films
2012.9	A molecular dynamics study of Hras-GTP complex and Hras-GDP complex
2011.3	Study on magnetic anisotropy and its electric field modulation in the surface and interface: from a first principles approach
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