International Symposium on Computational Science 2019
February 21, 2019
Kanazawa University, Japan

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Venue Natural Science and Technology Hall 5, building C4

- Oral presentations: Lecture room **6**
- Poster presentations: Lecture room **2**

Kanazawa University, Japan (Kakuma campus)
Kakuma-machi, Kanazawa 920-1192

URL http://polaris.s.kanazawa-u.ac.jp/iscs2019/

14:00 – 14:05 Opening (room **6**)

Invited lectures (25min + 5min Q&A)

14:05 – 14:35 Reza Rendian Septiawan (Bandung Institute of Technology)
An ODE control system of a rigid body on an ocean wave for a surfer simulation in the SPH method

14:35 – 15:05 Dam Hieu Chi (JAIST)
Mining Materials Data

15:05 – 15:20 Break

15:20 – 16:40 Short presentations (25 x 3min)

16:45 – 18:00 Poster session (room **2**)

List of short presentations

1. Muhamad Nasruddin Manaf (Kanazawa University)
   Origin of a Negative Fermi Contact Term of Anomalous Muonium in Silicon: First-Principles Study

2. Fathiyya Izzatun Az Zahra (Kanazawa University)
   Investigation Spherical Complex Desgin of Finite Unitary Reflection Group

3. Phansphitcha Gugaew (Kanazawa University)
   Numerical Study of Stem Cell Growth Model

4. Afrioni Roma Rio (Kanazawa University)
   Effect of External Magnetic Field to the Perpendicular Magnetic Thin Films from First-Principles Approach

5. Uswatun Hasanah (Bandung Institute of Technology, Kanazawa University)
   Solving matrix-valued convection problems using the generalized Lie derivative

6. Imam Wijaya (Kanazawa University)
   Stability estimates and a Lagrange-Galerkin scheme for a Navier-Stokes type model of flow in non-homogeneous porous media

7. Radhinka Bagaskara (Kanazawa University)
   Accelerating Molecular Dynamics Simulation with Parallel Computation

8. Arwansyah Muhammad Saleh (Kanazawa University)
   Theoretical Study on Stability of RA-VII for Anti-Cancer Agent by Molecular Docking and Molecular Dynamics Simulation

9. Thomas Aquino Ariasoca (Kanazawa University)
   First-principles calculation of hydrogen adsorption on graphene and silicene

10. Marleni Wirmas (Kanazawa University)
    First-principles study on electronic and optical properties of Titanium Dioxide: DFT and QSGW method

11. Afifah Maya Iknaningrum (Kanazawa University)
    3D simulation of Navier-Stokes flows in straight and curved cylindrical domain

12. Rifky Syariati (Kanazawa University)
    Large Anomalous Nernst Effect in The Ferromagnetic 1-T MnSe2

13. Yuto Aizawa (Kanazawa University)
    Mathematical formulation of neural network and deep learning algorithm

14. Monika Nur (Kanazawa University)
    Structural Study of Surface Alloys on Ag(111) Surface Through Density Functional Theory

15. Tharana Yosprakob (Kanazawa University and Chulalongkorn University)
Cahn-Hilliard Equation with Pattern Control

16. Ahmad Fauzan Fibriansyah (Kanazawa University)
Ring of the weight enumerator of triply even codes

17. Henokh Lugo Hariyanto (Kanazawa University)
Numerical study of vortex interactions in hyperbolic Ginzburg-Landau-type equation

18. Yuto Tanaka (Kanazawa University)
First-principles calculation on thermoelectric properties of group-V two-dimensional materials

19. Ramadhan Paninggalih (Bandung Institute Of Technology / Kanazawa University)
Numerical Level Set Method For Heat Equation With A Codimension One Source

20. Hana Pratiwi Kadarisman (Kanazawa University)
First-principles calculation of gallium monovacancy in gallium nitride

21. Nuntanut Foosarmpok (Chulalongkorn University, Kanazawa University)
A Comparison of Methods for the European Option Pricing

22. Md. Masum Murshed (Kanazawa University, University of Rajshahi)
A study on the stability of the shallow water equations with a transmission boundary condition in terms of energy estimates

23. Mutiara Dewi Lestari (Kanazawa University)
Theoritical Study on Dynamics of Vesicle by a Coarse-grained Model

24. Achmad Maulana Gani (Kanazawa University)
Investigation of magnetic field effects in solid α-oxygen using van der Waals density functional approach

25. Habibi Azka Nasution (Kanazawa University)
Theoretical Study of Bubble Dynamics by Coarse-Grained Model

An ODE control system of a rigid body on an ocean wave for a surfer simulation in the SPH method

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In this work we use a smoothed particle hydrodynamics (SPH) method coupled with a rigid body simulation to simulate a surfing board on top of an ocean wave. External forces are applied to the board to represent a surfer trying to control a surfing board. An ordinary differential equation (ODE) control is used to manipulate the external forces based on a position, velocity, and an inclination angle of the surfing board. The control system successfully helps the surfing board to move to and maintain its desired position.

Keywords: ODE, rigid body simulation, smoothed particle hydrodynamics, surfing board simulation.

Mining materials data

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Data mining is a broad discipline that aims to develop and use methods for extracting meaningful information and knowledge from large data sets. Recently, data mining methods have successfully been employed to the field of computational materials science. In this work, through examples, we demonstrate that data mining techniques can be used to automatically extract practical knowledge of chemical physics from materials systems. A predictive data mining approach can be applied to first-principles calculation data to computationally model the chemical and physical properties of materials with high accuracy and low computational cost [1,2]. A descriptive data mining approach can be used to obtain interpretable insights into the actuating mechanisms of physical phenomena from experimental and first-principles calculation data [3]. Further, combinations of the two approaches can be used to support the materials design process [4]. We also discuss the foundation and future of this research direction from both mathematical and physical/chemical perspectives.

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Origin of a Negative Fermi Contact Term of Anomalous Muonium in Silicon: First-Principles Study

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The study of defects in materials has been attracting scientific interest during the last three decades [1]. The study significantly contributes to the development of electronic devices. Hydrogen is one of the essential impurities in materials, especially in semiconductors [2]. Hydrogen can induce an unfavorable effect such as passivation of the shallow acceptor and donor, which reduces the performance of semiconductor devices [2,3]. On the other hand, hydrogen is in some cases a shallow impurity, which gives a favorable effect [4]. Muon spin resonance (μSR) is a useful tool to study hydrogen in materials [5]. The muon is an elementary particle whose mass is 1/9 of that of proton. The muon in a semiconductor captures the electron and forms muonium. The muonium has similarities with hydrogen. Therefore, the μSR can predict the dynamics of hydrogen in materials. Muonium in silicon is one of the most intensively studied systems [6,7]. Anomalous muonium in silicon was found to be located at the center of the bond and it has a negative value of the Fermi contact interaction (FCI). Previous theoretical studies presented large deviation from the experimental data and has not well explained the origin of the negative value of the FCI [3,8]. In this paper, we well reproduce the experimental value of FCI; the deviation from the experimental data is about 0.2 MHz [9]. We investigate the origin of negative value of FCI by considering a linear tri-hydrogen molecule, which is a simplified model of the present system.

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Investigation Complex Spherical Designs of Finite Unitary Reflection Groups

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Unitary group generated by reflectiom (u.g.g.r.) G is considered as a group which can construct a complex spherical design if $\mathrm{Harm}(k,l)^G = \{0\}$. One way to check $\mathrm{Harm}(k,l)^G = \{0\}$ is by using dimension argument. In this research, the dimension of $\mathrm{Harm}(k,l)^G$ for u.g.g.r $G_4 - G_{37}$ is calculated by using a generating function for harmonic polynomials.

Numerical Study of Stem Cell Growth Models

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Abstract

Stem cells are the body's master cells. All other cells arise from stem cells, including blood cells, nerve cells and others. Many researchers and doctors hope stem cell studies can help many problems in the medical areas. In this study, we are interested in a stem cell growth which may be useful in various stem cell systems. We study the stem cell growth model by using numerical method to see its behaviour. Moreover, focusing on a specific effect of the shape of intermediate stem cells' region, we consider a reduced model. After that, we apply a special numerical technique to solve this reduced model. Then we present numerical examples which clearly illustrate the effect of the shape of region.

Effect of External Magnetic Field to the Perpendicular Magnetic Thin Films from First-Principles Approach

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In the present day, the size of recording devices becomes much smaller and that capables to save more information, compared to ten years ago. The researchers search for the best possibility to reduce the dimension of devices, since they increase the storage capacity and also keep the stability at room temperature. One of the solutions is to use materials that have a high perpendicular magnetic anisotropy (PMA). High PMA materials can overcome the thermal energy (K_BT) near room temperature. $L1_0$ FePt is well known as high PMA material. This material is a ferromagnetic state bellow the Currie temperature around 750 K and exhibits high coercivity.

Using a first-principles approach, we investigated the effect of external magnetic field for the systems Pt(x ML)/Fe(1 ML)/Pt(x ML) (x= 1, 5). In our approach, the variational functional energy contains both of spin-orbit and spin dipole interactions. This makes sense under the external magnetic field. Our computational results show that for x=1, the system has a magnetic moment which is 3.10 μ_B for Fe. This result is comparable with the experiment that has been conducted by S. Imada et al. [1]. They obtained the saturated magnetic moment around 2.7 μ_B. This slightly difference might be due to the typical features that the density functional theory (DFT) tends to enhance the magnetic moment. We also calculated the magnetic anisotropy energy (MAE) which is 7.48 meV/cell for x=1. For this system, at first we set the magnetic moment of system to an out-of-plane (perpendicular) orientation. And then, we applied the external magnetic field ($\mathbf{H_x}$) along the in-plane orientation (x-direction). We chose several values of $\mathbf{H_x}$ up to 100 Tesla (T), we found that magnetic moment is saturated at around 60 T. From our analysis, the total energy difference (ΔE) respect to $\mathbf{H_x}$, we found that MAE is comparable to the energy at the critical point where the magnetic moment can be oriented to the in-plane orientation. We also investigated the Zeeman energy of system and found that after the critical point, the differences between Zeeman energies and ΔE are comparable to the MAE. We also did the same investigation for the x=5 system and found that the magnetic moment which is 2.92 μ_B for Fe. This value is smaller than that of x=1. The MAE for the x=5 system, which is 1.42 meV/cell, becomes five times smaller than that of x=1. This behavior of thickness dependence of Pt layers can be interesting for creating the best device needed in a different kind of application.

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Solving matrix-valued convection problems using the generalized Lie derivative

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In this work we recall the mathematical theory of the generalized Lie derivative and apply the idea of the generalized Lie derivative to find the approximate solution of matrix-valued convection problems. It is noted that a matrix-valued convection equation often appears in a system of viscoelastic flow model. Here, two-dimensional numerical examples are given to see the convergence order.

Key words: *generalized Lie derivative, matrix-valued convection problems*

Stability estimates and a Lagrange-Galerkin scheme for a Navier-Stokes type model of flow in non-homogeneous porous media

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The purposes of this work are to study the L^2 -stability of a Navier--Stokes type equation for non-stationary flow in non-homogeneous porous media proposed by Hsu and Cheng in 1989 and to develop a Lagrange--Galerkin scheme with the Adams--Bashforth method to solve that model numerically. The stability estimate is obtained thanks to the presence of a nonlinear drag force term in the model which corresponds to the Forchheimer term. We derive the Lagrange--Galerkin scheme by extending the idea of the method of characteristics to overcome the difficulty which comes from the non-homogeneous porosity. Numerical experiments are conducted to investigate the experimental order of convergence of the scheme. In both simple and complex designs of porosities, our numerical simulations exhibit natural flow profiles which well describe the flow in non-homogeneous porous media.

Accelerating Molecular Dynamics Simulation with Parallel Computation

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Molecular dynamics simulation is a method to simulate statistical and dynamical properties of particles in a system. The system allows us to observe the interactions among particles during a period of time. In order to obtain the best result, the system requires a large number (N) of particles and a smaller time step (Δt) in each iteration. However, this could produce longer computational time that the simulation is inefficient. To solve this problem, one of methods is to use parallel algorithms to optimize the computational time. By combining Nvidia's graphical processing units (GPUs) and CUDA application programming interface (API), we can build a molecular dynamics code with parallel algorithm that can maximize the number of particles and time step while running the simulation more efficiently.

A classical three dimensional molecular dynamics simulation was used in this research. To determine the particle's initial positions, we used the Box-Muller transformation method in order to randomly generate each set of initial coordinate. The integration algorithm of velocity Verlet was used to updates the position and velocity. The velocity Verlet method is well known as its stability and simplicity. The periodic boundary condition was used for the cubic simulation cell. The Lennard-Jones was used to describes the potential between particles. The forces, derivatives with respect to the position, is used to update the positions and velocities in conjunction with the velocity Verlet method. The computational amount in force calculation is proportional to N^2. CUDA is a method developed by Nvidia to write and run parallel programming. CUDA can be used on Nvidia's own brand GPUs. It's mainly used to parallelizing the force calculation, as it's the most taxing portion of the whole algorithm.

For the tests, we performed the benchmark between two programs, one running on serial algorithm while the other one is running on parallel algorithm using CUDA. We benchmark the overall running time of both programs. Within each test we also increased the number of atoms with the power of 2 (2^n) starting with 1024 atoms. The Δt is 0.01 second in 1000 steps. On 4096 atoms, the serial program took about 3,191.215 seconds to finish while the CUDA program 377.365 seconds to finish, roughly about 8 times faster. This research shows that by using parallel computation we able to greatly speed up the computation performance. However, there are still rooms for improvements. In the future, a further research is needed to add more potential interactions to the algorithms, such as intramolecular interaction, Van der Waals interaction, and Heisenberg interaction.

Theoretical Study on Stability of RA-VII for Anti-Cancer Agent by Molecular Docking and Molecular Dynamics Simulation

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1. Introduction

RA-VII is a bicyclic hexapeptide isolated from *Rubia cordifolia* and *R. akane* (Rubiacea*e*) [1,2]. This peptide has an anti-tumor activity by inhibiting the protein synthesis in the ribosome [3]. The 60S ribosome catalyzes the peptide bond formation and contains the polypeptide exit tunnel which is involved in the protein synthesis in cells [4]. Therefore, it become a potential target for tumor therapy by inhibiting its activity in protein translation mechanism. In this research, we performed molecular docking and molecular dynamics studies to accurately predict the cytotoxic mechanism of RA-VII as a promising drug for anti-cancer agent.

2. Methods

Molecular docking simulation was performed by using the AutoDock Vina packages with the Lamarckian genetic algorithm. Then, we performed molecular dynamics simulation to check the conformation of RA-VII in complex with the partial 60S ribosomal subunit. The energy representation (ER) method developed by Matubayashi group was used to estimate the solvation free energy ($\Delta\mu^{ex}$) between the partial 60S ribosome and RA-VII [5].

3. Results and Discussion

The structure of RA-VII was optimized to a structure with each constituent atom being a good relative spatial arrangement [6]. The docking simulation showed that binding models of RA-VII bound to 60S ribosomal subunit at different locations and had different structure each other. We found that the mode 1 had the lowest docking energy score as -16 kcal/mol. We performed molecular dynamics simulations to validate the conformation of RA-VII in the partial 60S ribosomal subunit during the simulations. Table 1 shows the average of the solvation free energy between the partial 60S ribosome and the RA-VII molecule. From our calculation, we obtained that RA-VII molecule corresponding to model 1, model 2, and model 5 are stable in binding with the partial 60S ribosome because the solvation free energy of each of those complexes become larger than the values of the standard deviations. Meanwhile, model 2 shows the highest value of the solvation free energy between the complex. It means that the RA-VII molecules of model 2 is not easy to leave from the binding pocket of the partial 60S ribosome by comparing other models.

Table 1. The average of $\Delta\boldsymbol{\mu}^{\boldsymbol{ex}}$ of the partial 60S ribosome in complex with RA-VII molecule

Model	Calculated $\boldsymbol{\mu}^{\boldsymbol{ex}}$ (kcal/mol)			$\Delta\boldsymbol{\mu}^{\boldsymbol{ex}}$
	Partial 60S Rib/RA-VII	Partial 60S Rib	RA- VII	
Model 1	-3057.22 (37.28)	-3090.48 (35.97)	51.52 (3.99)	-18.26 (2.67)
Model 2	-7387.87 (129.57)	-7387.88 (137.16)	56.50 (4.51)	-56.49 (12.11)
Model 5	-2727.95 (84.83)	-2751.59 (83.16)	52.11 (4.68)	-28.47 (3.01)

*Keyword*s: RA-VII molecule, 60S ribosome, molecular docking, MD simulations, solvation free energy

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First-principles calculation of hydrogen adsorption on graphene and silicene

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It has been known that partially hydrogenated graphene and silicene induce ferromagnetism, whereas fully hydrogenated system will not induce any magnetism. In this regard, we use first-principles calculations to investigate the stability and magnetic properties of graphene and silicene by considering various hydrogen adsorption configuration. First, we consider hydrogen monomer system to vary the supercell size. In this work, we use $3 \times 3 \times 1$,$4 \times 4 \times 1$, and $5 \times 5 \times 1$ supercells. In monohydrogen in silicene, we consider two hydrogen adatom positions: T position (on top of upper Si atom) and V position (on top of lower Si atom). Based on adsorption energy calculation, it is found that T-position is the most stable for hydrogen monomer. We found that for the hydrogen monomer in graphene and silicene, the magnetic moments are 1 μ_B. Next, we study hydrogen dimers. For both graphene and silicene, when two hydrogen atoms adsorb the same sublattices, the magnetic moment is 2 μ_B. On the other hand, when two hydrogen atoms adsorb different sublattices, any magnetism is not induced.

Keywords: DFT, graphene, silicene, hydrogen adsorption

First-Principles Study on Electronic and Optical Properties of Titanium Dioxide: DFT and QSGW methods

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Titanium Oxide (TiO_2) is recognized for its wide-range of practical use as photovoltaic solar cells, conventional catalyst support, photocatalytic substrate, and photoelectrochemical materials. It is considered as wide-gap semiconductor with long-term stability, non-toxic environmental and low-cost availability. Among the polymorphous TiO_2 structures, anatase and rutile structure are the most stable and synthesizable crystalline that are found in nature[1]. As the part of photovoltaic solar cell, electrons from valence band could be excited to conduction band form the process of photovoltaic effect. Therefore, band gap is one of the significant properties of this material. One of its application is Dye-sensitized solar cell (DSSC), where porous layer of TiO_2 is used as anode in the device. The sunlight can pass through this dye-layered TiO_2 where it can excite electron, transported in electrolyte, and produce some electrical current.

First-Principles calculation were carried out using density functional theory (DFT) on both structures. However, the band-gap results were found to be underestimated compared to the experimental result. Previous studies of DFT method also found this same specific problem[2]. To overcome these difficulties, we used a post-DFT method, called QSGW (Quasi-particle Self-consistent GW) method, which is a better approach than a usual GW method. It uses a self-consistent treatment (effective exchange correlation potential) to produce an optimum eigenvalue and eigenfunction of quasi-particle state[3], so that the band gap would be enhanced.

In this study, we present a combined approach of density functional approach and QSGW approach on the electronic and optical properties of TiO_2 in anatase and rutile structure. The fully optimized structures, obtained by minimizing the total energy and atomic forces (by varying lattice constants) are in good agreement with experiment. Optimized lattice constants are $a = 3.782$ Å and $c/a = 2.515$ (experiment $a = 3.784$ Å, $c/a = 2.512$) for anatase, and $a = 4.623$ Å, $c/a = 0.646$ (experiment $a = 4.594$ Å, $c/a = 0.644$) for rutile. We calculated band dispersions, density of states, and dielectric function of both structures. As expected, the band gaps from QSGW are much more enhanced compared with those of usual DFT method, but they are overestimated compared with the experimental result. This features are consistent with other cases[4]. This discrepancy between both methods were also investigated, especially in band dispersion. The better result could be taken into account when calculating the surface properties of TiO_2.

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3D simulation of Navier-Stokes flows in straight and curved cylindrical domains

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Research about natural violent flow phenomena like tornado has been done by researchers using numerical simulations, where Finite Element Method (FEM) was used to perform numerical computation of axisymmetric Navier-Stokes flows with no-slip flat boundary in a straight cylindrical domain which correspond to an ideal shaped tornado [1]. But in natural phenomena, the central axis of tornado might have curvature. Using similar numerical approach, we make 3D simulations in curved cylindrical domain to simulate the tornado with curvature. From the result, it is observed that for several pairs of straight and curved cylindrical domain shape and initial condition, the effect of the domain shape is larger compared to the effect of the initial condition. It is also found that for the larger curvature, the distance from the position of maximum magnitude of the velocity to the central axis is getting larger.

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Large Anomalous Nernst Effect in The Ferromagnetic 1-T $MnSe_2$

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Abstract

The two-dimensional 1-T $MnSe_2$ has been discovered experimentally by using molecular beam epitaxy (MBE) in 2018 [1]. This material has essential properties, and it answers the challenge about the room temperature two-dimensional ferromagnetic material [1,2]. It has not only high Curie temperature, but also it has perpendicular magnetic anisotropy which favorable for thermoelectric based on the anomalous Nernst effect (ANE). By using the first-principles calculation, we found that the ANE coefficient is -3.74 μV/K on the Fermi level at 300 K. This result shows that the 1-T $MnSe_2$ has large ANE coefficient which can be a candidate for new generation of thermoelectric devices.

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Matheamtical formulation of neural network and deep learning algorithm

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The machine learning, especially so called the deep learning, is recently widely used in industry and sciences. However, its mathematical formulation is often omitted in many application-oriented literatures. We give a brief review on the mathematical formulations for tne neural network and deep learning algorithm, and compare the difference in the number of nodes numerically.

Structural Study of Surface Alloys on Ag(111) Surface Through Density Functional Theory

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Surface alloys are synthesized by depositing atoms into surfaces, and has attracted much attention recently due to application, for example, spintronics [1]. Metal-semiconductor interface is of great importance in industry, and, for instance, an Si/Ag interface is a promising candidate for solar cells [2]. Many kinds of surface alloys has been studied: for example, Ge/Ag(111) [3], Ag/Si(111) [4], Pb/Ag(111) [5], Bi/Ag(111) [6], Sn/Ag(111) [7]. Such structural studies of surface alloys may provide important information to forming metal-semiconductor and metal-metal interfaces.

In this study, we have investigated *M*/Ag(111) surface alloys systematically, where *M* is group III, IV, and V atoms, B, Al, Ga, In, Tl, C, Si, Ge, Sn, Pb, N, P, As, Sb, and Bi. We focused on the corrugation parameter defined by the height of *M* atoms from the Ag atoms in the top atomic plane. We used OpenMX code [8] and performed first-principles calculation for *M*/Ag(111) surface alloys. We will discuss *M*-atom dependence of corrugation parameters.

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Cahn-Hilliard Equation with Pattern Control

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In this work, we are interested in pattern control of phase separation described by the Cahn-Hilliard equation. The volume preservation, energy decay property, and a stability estimate are presented. Then, we establish the time semi-discrete scheme. Consequently, to compare the discrete scheme with the Cahn-Hilliard equation, we show error estimates and our convergence theorem. Moreover, we construct different patterns of phase separation in two-dimension in the numerical results.

Ring of the weight enumerators of triply even codes

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Abstract. We determine the ring of the weight enumerators of triply even codes which contain all one vector for small genus.

Numerical study of vortex interactions in hyperbolic Ginzburg-Landau-type equation

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The interaction of several vortices for 2D and 3D cases in hyperbolic Ginzburg-Landau-type equation (HGLE) are investigated numerically. By using explicit scheme, it provides stable scheme for solving HGLE in a rectangular domain with a specific initial data and Dirichlet boundary condition. Several initial data of vortex point(s), vortex line(s), and vortex ring(s) are used to study the behaviour of vortex interactions. We find that the initial data of two vortex points with winding number $w = \pm 1$ behaves like point charge particles. Similar situation happens in 3d cases when we consider two vortex lines and two vortex rings. There are also interesting behaviour when we generate randomly the position of vortices with their winding number $+1$ or -1. The remaining number of vortices after time T depend on the total winding number. Further works are focused on the building of mathematical framework for the vortex interaction above.

First-principles calculation on thermoelectric properties of group-V two-dimensional materials

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Thermoelectric materials, which can convert heat energy to electric energy, have attracted much interests owing to energy issues. To achieve high-performance thermoelectric conversion, we need high electric conductivities, large Seebeck coefficients and low thermal conductivities. Low-dimensional and nanostructured materials could be new candidates for efficient thermoelectric conversion [1-3]. The nonequilibrium Green's function (NEGF) method [4] is suitable for investigating the transport properties of such nanostructured systems. We focus on group-V two-dimensional (2D) materials. We perform first-principles calculations by using NEGF method to investigate the spin-orbit coupling (SOC) effect on the thermoelectric properties in α-bismuthene[5], which is the (110) bilayer of bismuth, and clarify the origin of the anisotropic thermoelectric preterites.

Figure 1 shows the phonon transmittance $\zeta_p(\omega)$ and the electron transmittance $\zeta_e(E)$ of α-bismuthene. We find anisotropic behaviors in electron and phonon transmittance. Both $\zeta_p(\omega)$ and $\zeta_e(E)$ in the zigzag (ZZ) direction are larger than those in the armchair (AM) direction. The anisotropy is explained on the basis of the number of transport channels in each direction. The anisotropy in the thermoelectric properties originates from the anisotropic transmittance. We include the SOC effect in the transmittance calculations and find that $\zeta_p(\omega)$ and $\zeta_e(E)$ are affected by the SOC. Then, we calculate the thermoelectric properties by using the transmittance and estimate the figure of merit ZT for thermoelectric performance. As shown in Fig. 2, the peak values of ZT in α-bismuthene are enhanced by the SOC. The peak values of ZT are 0.49 and 1.63 in the non-SOC calculation and the SOC calculation, respectively.

In conclusion, we found that the anisotropy in the thermoelectric properties of α-bismuthene originates from the anisotropic transmittance explained on the basis of the difference of the number of transport channels. We include the SOC effect in our calculations and clarify that the SOC has a substantial effect on ZT of α-bismuthene.

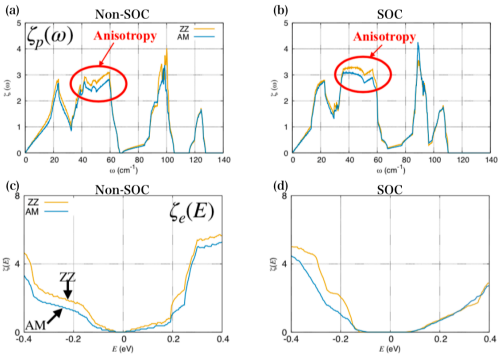

Figure 1: Transmittance of α-bismuthene. (a) and (b) : Phonon transmittance. (c) and (d) : electron transmittance.

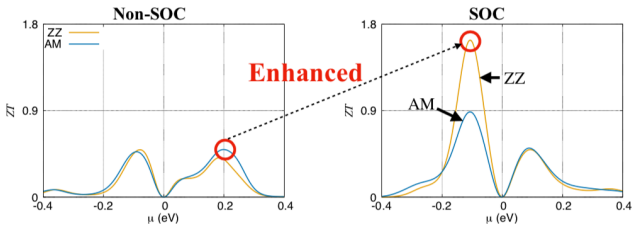

Figure 2: Figure of merit ZT of α-bismuthene at 300 K.

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Numerical Level Set Method For the Heat Equation With a Codimension One Source

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Abstract

The research motivation comes from phase transition phenomena, for example crystal growth. The evolution of heat can be described by the heat equation with a source concentrated on a curve or a surface, where the crystal surface becomes the heat source. The research goal is to introduce a numerical method for this problem. We use the Poisson equation with a curve heat source as a test problem and apply the finite element method using the FEniCS library for the implementation. The right-hand side of the weak form becomes a surface integral and can be expressed in three ways adapted mesh, point sources and a level set method. Adapted mesh and point sources are supported by FEniCS but the level set method is not (research contribution). We compare error and time cost of the three methods.

First-principles calculation of gallium monovacancy in gallium nitride

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Gallium nitride is a wide band gap semiconductor (Eg=3.47 eV) [1]. The Ga monovacancy (V_{Ga}) in GaN affects the physical properties of the GaN. In this paper, we carry out calculations of gallium monovacancy in GaN based on the density functional theory. We study the spin-polarized state in the gallium monovacancy system. By using the calculated lattice constant of the bulk, we construct the supercell to simulate the Ga monovacancy. In the optimized geometry, the four N atoms near the vacancy site are displaced outwardly. The calculated magnetic moment is $3\mu_B$. By calculating the spin density distributions in the real space, we find that the majority spin is localized and the minority is delocalized. We also find that the positron lifetime for the majority spin is shorter than that of the minority spin.

Keyword: GaN, monovacancy, spin-polarization, geometry, positron, annihilation, lifetime.

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A Comparison of Methods for The European Option Pricing

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Abstract

The derivative securities are important in financial industries as they perform remarkable risk and profit management. One of the derivative securities is option. In this work, we focus an option in European type and its properties. Additionally, we approximate the European option pricing with two methods, which are the Black-Scholes formula and the Monte Carlo simulation, by a numerical approach. We found that both of the results are in agreement.

A study on the stability of the shallow water equations with a transmission boundary condition in terms of energy estimates

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In this study, the stability of the shallow water equations (SWEs) with a transmission boundary condition is studied theoretically and numerically. For a suitable energy, some mathematical results are derived to confirm the stability of the SWEs with the Dirichlet and the slip boundary conditions. Based on the mathematical results, the stability of SWEs with the transmission boundary condition is also confirmed numerically by finite difference method (FDM) in terms of the energy. From the numerical results, it is found that for the transmission boundary condition the total energy decays with respect to time.

Theoritical Study on Dynamics of Vesicle by a Coarse-grained Model

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Membranes are ubiquitous in nature, and are essential for cellular life. Many crucial biological functions take place at or near membranes. Vesicles are a model system used to study the dynamic behaviour of biological cells, similiar in some respects to red blood cells. A vesicle is a droplet of viscous fluid encapsulated by a phospholipid bilayer membrane suspended in a fluid of either the same or different viscocity as the inner one. Both the volume and the surface area of the vesicle is conserved. In this work, motion of membrane particle performs Brownian motion. The theory of Brownian motion is used to approximate the dynamics of nonequilibrium systems. The fundamental equation is called the Langevin equation. It contains both frictional forces and random forces. We have succeeded to perform simulation of vesicle using langevin dynamics equation with conserved volume and surface area.

Investigation of magnetic field effects in solid α-oxygen using van der Waals density functional approach

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Oxygen molecule, in the ground electronic state possesses nonzero spin (S=1), which makes the oxygen molecule a magnetic system. The low-temperature phase of solid α-oxygen is an electron-spin antiferromagnetic insulator consisting of single element. An analysis of the comprehensive magnetic field-temperature (H-T) phase diagram in solid oxygen indicates the possibility that there exist phases induced by a magnetic field. This makes solid oxygen an extremely interesting object [1,2]. A sudden increase in magnetization and in light transmission in the visible range is observed when pulsed magnetic fields greater than 90 T were applied. This findings indicate that the first-order phase transition from α-phase occur in ultrahigh magnetic fields and that there is a new phase θ-oxygen. In this research, we performed first-principles calculations on antiferromagnetic solid α-oxygen under external magnetic field and measured its magnetic properties.

In this calculation, we used the spin density functional theory (SDFT), fully relativistic ultra-soft pseudopotential plane-wave basis method, magnetic dipole contribution using spin density and two-spinols wave function [3]. We included spin-orbit interaction in this calculation with the exchange-correlation of conventional type (GGA) and spin polarized van der Waals density functional (vdW). The **k** point sampling of 8x8x8 mesh was used. Experimental lattice constant was referred from the neutron-diffraction measurement[4]. We applied the external magnetic field in the range of 0-100 T.

Our result shows that the magnetization is increased with the non linear behavior as the external magnetic field increases. The total spin magnetic momenta at 100 T are $0.307\mu_{\mathrm{B}}$ and $0.309\mu_{\mathrm{B}}$ in the x and z directions, respectively, for vdW. The GGA values were $0.368\mu_{\mathrm{B}}$ and $0.364\mu_{\mathrm{B}}$. The magnetization was fitted to the 4th order polynomial function of external field. The susceptibility component ($\chi^{\alpha\beta}$), where α and $\beta = \mathrm{x}, \mathrm{y}, \mathrm{z}$, was calculated from the first derivative of polynomial function. The value of χ^{xx}, χ^{yy}, χ^{zz} at zero field were 2.755×10^{-3}, 0, and $2.777 \times 10^{-3}\mu_{\mathrm{B}}$/T, for vdW. χ^{xx}, χ^{yy}, χ^{zz} were 3.094×10^{-3} , 0, and $3.079 \times 10^{-3}\mu_{\mathrm{B}}$/T for GGA values. The uniform susceptibility (χ_{uni}) is obtained by taking the average of the diagonal components. The obtained values were 1.844×10^{-3} and $2.058 \times 10^{-3}\mu_{\mathrm{B}}$/T for vdW and GGA, respectively. The χ_{uni} is slightly larger for the GGA compared to vdW. Those values are smaller than the experiment [2]. The difference may come from several factors, such as the lack of treatment of Landau diagmanetism, susceptibility contribution from orbital moment and underestimation in the bandgap. The present results imply that we can combine SDFT with the external magnetic field in order to calculate magnetic properties such as magnetization curve and susceptibility.

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Theoretical Study of Bubble Dynamics by Coarse-Grained Model

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It is interesting to study the biological system. One of them is how to describe a surface of the system. In this work, we simulate on the dynamics of system surface, where the system that we propose is a bubble system. In this study, we solve the Langevin equation of motion to approach the bubble system. We have two potential energy function V_1 and V_2 for our bubble dynamics. Then, we used Taylor's expansion as an approach to numerical calculations. First, we simulated the surface of the bubble system with a fixed configuration. Second, we simulated the surface of the bubble system with a changed configuration. Surface transition systems such as bubble systems has been proposed. In this study, the Langevin equation which has a potential function as the principle of minimization of surface area and volume conservation can be implemented.