International Joint Symposium on Computational Science

March 3-7, 2008

Institute of Technology Bandung and Kanazawa University

Incubation Center 1F, Seminar Room,

Kanazawa University

International Joint Symposium on Computational Science

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Opening Ceremony: Afternoon, March 3

Part 1: Mathematics: Morning, March 4

Part 2: Physics, Chemistry, Biology and Earth Science: Afternoon, March 4, March 6-7

Incubation Center 1F, Seminar Room, Kanazawa University

Opening Ceremony

Monday, March 3

15:00 Koji Nakamura,

History of collaboration between Institute of Technology Bandung and Kanazawa University

15:10 Yujiro Hayashi, President of Kanazawa University

15:15 Djoko Santoso, Rector of Institute of Technology, Bandung

15:20-15:30 Break

15:30 Djoko Santoso, Rector of Institute of Technology, Bandung

16:15 Akhmaloka, Dean of the Faculty of Science, Institute Technology Bandung

17:00 End of opening ceremony

Part 1 Program

Tuesday, March 4

Chair: Katsuyoshi Ohara

9:00 Opening

9:10 [4A1] Kenichi Kawagoe, On limits of the polynomial invariants of knots and links

9:40 [4A2] Tatsuro Ito, Algebraic combinatorics: a personal overview

10:10 [4A3] Paul Terwilliger, Tridiagonal pairs and the quantum affine algebra $U_q(\widehat{sl}_2)$

10:40--10:50 Break

Chair: Tatsuro Ito

10:50 [4A4] Atsushi Kasue, Compactifications of infinite graphs and p-Dirichlet energy

11:20 [4A5] Invited Talk

Edy T. Baskoro, Ramsey Numbers, Edge-Magic Total Labelings and Secret Sharing Schemes

12:00 End of morning session

Part 2 Program

Tuesday, March 4

Chair: Masahide Sato

14:00 [4P1] Invited Talk:

Mahasena Putra, Population Synthesis of Cataclysmic Variable Stars

14:40 [4P2] Invited Talk:

Suprijadi, Heat flow control system using intelligence algorithm

15:20 end of session

Thursday, March 6

Chair: Tatsuki Oda

9:30 [6A1] Mineo Saito, Quantum Mechanical Simulation of Electronic Structures of Defects in Carbon Materials

10:00 [6A2] Fumiyuki Ishii, First-principles Simulation of Ferroelectrics

10:30-10:40 Break

Chair: Masako Takasu

10:40 [6A3] Koji Nakamura, Long-term Dynamics of Insects Populations

under Different Climate Conditions in Indonesia

11:20 [6A4] Christopher Yanto, Beetle (Coleoptera) Assemblages at Four Different Habitats in Mount Tangkuban Parahu Area, West Java-Indonesia

11:35 [6A5] Indah Trisnawati, Diversity and Structure of Above-ground Arthropod Assemblages During the Restoration of Satoyama in Kanazawa, Japan

11:50 [6A6] Ida Kinasih, Composition and Structure of Litter and Soil Macrofauna Communities in Satoyama Region in Kanazawa, Japan

12:05 [6A7] Ramadhani Eka Putra, Changes of Local Pollination Ecology during Restoration of Satoyama System

12:20- Lunch Break

Afternoon Session

Chair: Mineo Saito

14:00 [6P1] Kazue Tazaki and Siti Khodijah Chaerun,

Heavy oil spill accidents in Japan, Korea and Indonesia: International joint project between Kanazawa University and Bandung Institute Technology.

14:40 [6P2] Invited Talk

Sukirno, The Research Road Map of Physics of Electronics and Materials, Research Group of ITB

15:20-15:40 Break

Chair: Fumiyuki Ishii

15:40 [6P3] Tatsuki Oda,

First-principles Molecular Dynamics Method with Noncollinear Magnetism

16:10 [6P4] Akihiko Hosokawa, Development of fully relativistic pseudopotentials and application to the sixth-row elements of the periodic table

16:25 [6P5] Masahito Tsujikawa, Electronic structures and magnetic anisotropies

of thin iron films on platinum surfaces

16:40 End of Session

Friday, March 7

Chair: Acep Purqon

9:30 [7A1] Masahide Sato, Instabilities of Steps on a Vicinal Face

10:00 [7A2] Shinichi Miura, Chemical Processes in the Superfluid Helium

10:30-10:50 Break

Chair: Shinichi Miura

10:50 [7A3] Kiyoshi Nishikawa, Reviews on the quantum control of molecular system

11:20- [7A4] Acep Purqon, Measuring Disordered degree in Shape Fluctuation of Few Correlated Phospholipids

11:35 [7A5] Noriyoshi Ohta, Brownian Dynamics Simulation of Polyimide Gel

11:50- Lunch Break

Afternoon session:

Chair Kiyoshi Nishikawa

14:00 [7P1] Invited Talk

Muhamad A. Martoprawiro, Ab initio Quantum Chemical Study of the Thermal Decomposition of Aromatic Substituted N-acylhydrazones and N-thioacylhydrazones

14:40 [7P2] Kazunaka Endo, Spectral Simulation of Carbon Allotropes

15:10 [7P3] Tomonori Ida, Theoretical Auger spectra of molecule by two-electron propagator method

15:40 End of session

4A1

On limits of the polynomial invariants of knots and links

Kenichi Kawagoe

After Kashaev's experimental confirmation [2], it seems that there is a connection with the colored Jones polynomial for a knot K and certain geometric invariants of K. Let $J_N(L;q)$ be the colored Jones polynomials of associated with the N-dimensional irreducible representation of the quantum group $U_q(\mathfrak{sl}(2,\mathbb{C}))$. $J_N(L;q)$ is normalized by 1 for a trivial knot. We set $J_N(K) = J_N(K; \exp\frac{\sqrt{-1}}{N}\pi)$. Then, for any hyperbolic knot K, the following conjecture is suggested.

Conjecture 1 (Volume Conjecture)**.**

$$\lim_{N\to\infty} \frac{|\log J_N(K)|}{N} = \mathrm{vol}(\mathbb{S}^3 \setminus K).$$

This equality is very mysterious because the left hand side only depends on the topological structure, but the right hand side only depend on the hyperbolic structure. This conjecture is confirmed by some examples [2] [3] [4].

In this talk, for the Figure-eight knot and the Whitehead link, we study the volume conjecture by the HOMFLY polynomial [1] instead of the Jones polynomial. The HOMFLY polynomial $H(K;a,q)$ is a two variable extension of the Jones polynomial. We obtain the colored Jones polynomial from the HOMFLY polynomial by $J_N(K;q) = H_{2,N}(K;q^2,q) = H(K;q^2,q)$. (The original definition of the Jones polynomial corresponds to $N = 2$.) For the Figure-eight knot 4_1, we rigously obtain the following theorem.

Theorem 2.

$$0 \leq \lim_{N\to\infty} \frac{|\log H_{M,N}(4_1)|}{N} \leq \frac{2}{\pi}\int_{\frac{1}{6}\pi}^{\frac{5}{6}\pi} \log 2\sin x\, dx.$$

For the Whitehead link, we observe similar asympotic behavior in the case of the Figure-eight knot.

References

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Algebraic combinatorics: a personal overview

Tatsuro Ito

Abstract

I will give a personal overview of algebraic combinatorics. Algebraic combinatorics is a relatively young area, which took its present form in the middle of the 1970's during the efforts culminating in the complete classification of finite simple groups. Algebraic combinatorics is often called 'group theory without groups', accommodating a wider range of mathematical symmetries. Lately, this area has been developing rapidly, interacting with many other branches of mathematics such as low dimensional topology, mathematical physics, lattices, modular forms, operator algebras and random walks.

4A3

Tridiagonal pairs and the quantum affine algebra $U_q(\widehat{sl}_2)$

Tatsuro Ito and Paul Terwilliger

Abstract

Let $\mathbb{K}$ denote a field, and let V denote a vector space over $\mathbb{K}$ with finite positive dimension. We consider a pair of linear transformations $A : V \to V$ and $B : V \to V$ which satisfy the following two conditions:

1. There exists a basis for V with respect to which the matrix representing A is irreducible tridiagonal and the matrix representing B is diagonal.
2. There exists a basis for V with respect to which the matrix representing A is diagonal and the matrix representing B is irreducible tridiagonal.

We call such a pair a *Leonard pair* on V. In this talk we discuss a mild generalization of a Leonard pair known as a *tridiagonal pair*. Tridiagonal pairs arise naturally in the theory of Q-polynomial distance-regular graphs. We show how certain tridiagonal pairs give modules for the quantum affine algebra $U_q(\widehat{sl}_2)$.

Compactifications of infinite graphs and p-Dirichlet energy

Atsushi KASUE
Department of Mathematics, Kanazawa University

In this talk, we consider a connected, locally finite graph $G = (V, E)$ with vertex set V and edge set E, and discuss some geometric and potential theoretic properties of the graph.

When a positive function r on E is given, we are able to define a distance d_r on V by assigning a pair of points $x, y \in V$ the infimum of the length of curves joining them, where each edge $e \in E$ is of length $r(e)$. For the case: $r = 1$, the distance is called the graph distance of G.

There are a variety of compactifications of G. In fact, let Φ be a family of bounded functions on V, then there exists a (up to canonical homeomorphism) compact Hausdorff space $\mathcal{C}_\Phi(G)$ with the following properties: (1) V is embedded in $\mathcal{C}_\Phi(G)$ as an open and dense subset; (2) every function of Φ extends to a continuous function on $\mathcal{C}_\Phi(G)$; (3) the extended functions separate the points of the boundary $\partial\mathcal{C}_\Phi(G) = \mathcal{C}_\Phi(G) \setminus V$. We remark that if $\Phi \subset \Psi$, then tehre is a canonical continuous map of $\mathcal{C}_\Psi(G)$ onto $\mathcal{C}_\Phi(G)$

We are interested in families as follows: (i) the space $\mathcal{E}(G)$ of bounded functions on V that are locally constant outside a compact subset of V (the compactification is called the end compactification of G, denoted by $\mathcal{C}_\mathcal{E}(G)$); (ii) the space $\mathcal{BL}(G, r)$ of bounded Lipschitz functions with respect to the distance d_r; (iii) the p-Dirichlet space of G, $\mathcal{L}^{1,p}(G)$, consisting of functions on V with finite p-energy, where an exponent $p \in (1, +\infty)$. The closure of the subspace of finitely supported functions in $\mathcal{L}^{1,p}(G)$ will be denoted by $\mathcal{L}^{1,p}_0(G)$. The compactification associated with $\mathcal{L}^{1,p}(G)$ is called the p-Royden compactification of G and denoted by $\Re_p(G)$. There is an important part of the Royden p-boundary $\partial\Re_p(G) \setminus V$, called the p-harmonic boundary, which is defined by $\Delta_p(G) = \{x \in \partial\Re_p(G) \mid f(x) = 0, \quad \forall f \in \mathcal{L}^{1,p}_0(G)\}$. We note that $\mathcal{E}(G) \subset \mathcal{L}^{1,p}(G)$ for any p, and $\mathcal{BL}(G, r) \subset \mathcal{L}^{1,p}(G)$ if r is p-summable (i.e., $\sum_{e\in E} r(e)^p < +\infty$).

Given $p \in (1, +\infty)$ and a subfamily Φ of $\mathcal{L}^{1,p}(G)$, the identity map i of V extends to a surjective continuous map $I : \partial\Re_p(G) \to \partial\mathcal{C}_\Phi(G)$. Suppose the p-harmonic boundary is not empty, that is, G is not p-parabolic. Then we can show that the Dirichlet problem for p-Laplacian is solvable on $\Delta_p(G, \Phi) = I(\Delta_p(G))$, namely, for any continuous function u on $\Delta_p(G, \Phi)$, there exists a unique p-harmonic function H on V such that $\lim_{x\in V\to\xi} H(x) = u(\xi)$ for any $\xi \in \Delta_p(G, \Phi)$.

We remark that if G satisfies the strong isoperimetric inequality, then G is not p-parabolic and $\partial\Re_p(G) = \Delta_p(G)$ for all $p \in (1, +\infty)$, so that in this case, the Dirichlet problem is solvable on the boundary $\partial\mathcal{C}_\Phi(G)$; but it may occur that $\partial\mathcal{C}_\Phi(G)$ consists of a single point, even though $\Delta_p(G)$ is nontrivial.

Ramsey Numbers, Edge-Magic Total Labelings and Secret Sharing Schemes

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Ramsey theory was initially studied in the context of the problem of finding a regular procedure to determine the consistency of any given logical formula (1928). The theory became famous after Paul Erdös and George Szekeres (1935) applied it in graph theory. The idea behind Ramsey number is basically as follows. For graphs G and H, the notation of $F \to (G, H)$ denotes that in **any** 2-coloring on the edges of graph F there exists a mono-color G or H in F. A *(graph) Ramsey number* $R(G, H)$ is $\min\{n | K_n \to (G, H)\}$. Let $\mathfrak{R}(G, H) := \{F | F \to (G, H)$ and $F \backslash e \not\to (G, H)$ for any edge $e\}$. The graph $F \in \mathfrak{R}(G, H)$ is called a *Ramsey* (G, H)*-minimal graph*. The determination of Ramsey numbers $R(G, H)$ has been studied for various combinations of graphs G and H. However, there is no general formula of $R(G, H)$ for all G and H. In fact, the value of $R(G, H)$ depends heavily on the structures of G and H.

In this talk, we shall discuss the recent progress on the Ramsey numbers of wheels versus other graphs, as well as their disjoint unions. We are also interested in characterizing and enumerating all Ramsey-minimal graphs in $\mathfrak{R}(G, H)$ for simple graphs G and H.

An *edge-magic total labeling* on graph $G(V, E)$ with p vertices and q edges is a bijection $\lambda : V(G) \cup E(G) \to \{1, 2, \cdots, p + q\}$ so that there exists integer k satisfying

$$\lambda(x) + \lambda(xy) + \lambda(y) = k,$$

for each edge xy. The notion of edge-magic total labeling was firstly introduced by Sedláček (1963), and formulated by Kotzig and Rosa (1970). Deciding whether a given graph possesses an edge-magic total labeling or not is an NP-complete problem. Therefore, the study of determining this property for a particular class of graphs cannot be avoided.

In this talk, we investigate such labeling applied to some classes of graphs. We also investigate the critical sets of edge-magic labelings on some particular graphs, especially star, and the application on secret sharing scheme.

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Population Synthesis of Cataclysmic Variable Stars

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Abstract

A cataclysmic variable (CV) "star" is a system consisting of a white dwarf accreting mass from a companion star (late type, low mass). CVs are very interesting objects both from observational and theoretical point of view. The accretion processes in CVs have led to the development of accretion disk theories, after astronomers succeeded in interpreting puzzling observational data. From the point of view of stellar evolution, CVs are also very interesting objects, since their observables can be utilized to put constraints on the proposed scenarios of their formation. In this work, we report our attempt to perform a population synthesis of CVs. We use Monte Carlo method to choose initial parameters of the progenitor binaries, and calculate the necessary evolutions directly. There are parameters, some are in the evolution code and some are associated with the chosen scenario, that have to be fixed. At post common-envelope stage, we find a double peaked distribution of white dwarf masses and a distribution of λ (a quantity describing the structure of the primary star at the onset of the common envelope evolution) that is different from the often assumed value in the literature.

Heat flow control system using intelligence algorithm

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Abstract

Automatic control is becoming more and more important in this age of automation. The duty of control engineering is to bring these parameters to certain pre-defined values (set point), and to maintain them constant against all disturbing influences. During the past decade, electronic control unit has started to replace mechanical control unit, since it was believed to have a better performance and much simpler to design. Despite its rapid development, control system is still the biggest problem in all fields. This was caused because the difficulty level of a control system will increased according to the difficulty to solve a problem. The merge of control system with artificial intelligence was a method to simplify the difficulty level of designing a control system.

Many methods were proposed in artificial intelligence, Fuzzy Logic and expert system were popular choice. The methods are practical alternative for a variety of challenging control applications since it provides a convenient method for constructing nonlinear controllers via the use of heuristic information. On the other hand, heat flow is play an important role in several field, such as in health and medical problem, chemical industry, transportation engine or in our home. In this paper, the simulation of fuel flow control system in an engine aircraft using fuzzy logic and application of expert system in control heat transfer in isolated room were reported.

Keywords :
Heat transfer, fuzzy logic, expert system

Quantum Mechanical Simulation of Electronic Structures of Defects in Carbon Materials

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Drastic changes of almost all the fields in modern societies such as politics, economics and education originate from development of information technology. This technology is based on semiconductor technology that was initiated from discovery of transistor effects in 40's in the USA and has been developed by downsizing of semiconductor devices. However, so called Moore's law describing the fact that the transistor density in integrated circuits increases approximately double every two years suffers breakdown. Therefore nanotechnology that will replace the semiconductor technology attracts wide interests and is expected to be realized by using carbon nanotubes that was discovered in early 90's in Japan [1].

In these days, carbon nanotubes and graphene are extensively studied and prototypes of devices by use of these carbon materials are proposed by many groups. To realize carbon nanodevices, control of defects is crucially important. However, compared with the study in the field of semiconductors, the study of defects in carbon materials is still insufficient.

Computer simulations on the basis of quantum mechanics are necessary in the field of nanotechnology. In this paper, we perform quantum-mechanical electronic-structure calculations on defects in carbon materials. We have used two open codes、PHASE[2] and OpenMX[3].

We first study the most fundamental defects, vacancies (hole of atoms) and adatom (adsorbed atom). As for vacancies, hexavacancy having six-atom holes was expected to be stable, thus 6 is assigned to the magic number[4]. Considering atomic relaxation, we find that five-member rings are formed in all-size vacancies and that 2,4, and 6 are magic numbers. Then we expect that these vacancies are detected under some experimental conditions. The adatom dimmer also forms two pentagons and is very stable.Therefore, this defect is expected detected under the condition that adatom migrates.

We also study the graphene nanoribon which was found to show antiferromagnetism. We examine carrier doping effects and find that either electron doping or hole doping induces the ferromagnetism, therefore we demonstrate that the magnetic character of carbon materials can be controlled by means of carrier doping.

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First-Principles Simulation of Ferroelectrics

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The research on ferroelectric materials has been increasingly motivated by both basic scientific concerns and potential or practical applications over a wide variety of electronics and optics: nonvolatile memories, piezoelectric transducers/actuators, pyroelectric sensors, high performance gate insulators in field-effect transistors, nonlinear optics and so on. Therefore, coexisting of ferroelectricity and other novel functionality in materials would be quite important for new-type electronic and photonic devices of great current interest.

The recent observation of magnetoelectric (ME) effect in multiferroics with spiral or canted spin structure provides a novel approach to the mutual control of magnetization and electric polarization. Despite extensive experimental and theoretical studies, the origin of electric polarization remains still a controversial issue.

We have performed the first-principles calculations of electric polarization using Berry phase approach in several multiferroics with non-collinear magnetic structures. We found two possible mechanism of electric polarization induced by noncollinearity of spin instead of atomic displacement. One is spin-orbit origin of electronic polarization with spiral spin structure and the other is the change of Born effective charges with spin canting. In both cases, though there is still inversion symmetry in nuclear coordinate system, finite electric polarization can be obtained. These mechanisms are crucial to understand the magnetically driven ferroelectricity and ME effect, induction of electric polarization by a magnetic field.

This work was done in collaboration with K. Sawada, T. Ozaki, N. Nagaosa, and K. Terakura.

Long-term Dynamics of Insects Populations under Different Climate Conditions in Indonesia

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Since early 1980's, I have been involved in a series of Indonesia-Japan joint projects in which many researchers and students from various universities and institutions from both countries participated. In this opportunity, I will present some of my experience and research in Indonesia.

Indonesia has environmental conditions that are extremely diversified both physically and biologically. It has wide areas of tropical rainforest that harbor the world's richest and most diverse fauna and flora. Going eastwards from central Java to the Lesser Sunda Islands, however, the rainfall decreases and becomes distinctly seasonal, and vegetation changes correspondingly. Although air temperature is very constant in tropical environments, temporal fluctuation of rainfall is no more stable than that in temperate zones. In Indonesia, moreover, El Niño brings drier seasons and has occurred at an average interval of 4-5 years, but its periodicity and intensity have greatly changed from time to time. In recent decades, the impact of severe droughts associated with the 1982-1983 and 1997-1998 El Niños were extremely strong.

Since 1990, we have studied population dynamics of the phytophagous lady beetles, *Epilachna vigintioctopunctata*, *E. enneasticta* and *E*. sp. 3 (aff. *emarginata*), (Coleoptera: Epilachninae) on Padang, Sukarami (West Sumatra), Bogor (West Java) and Purwodadi (East Java), Indonesia. These sites have distinctly different climate conditions, e.g. Padang has a typical tropical rainforest climate without a clear alternation of wet and dry seasons, while Purwodadi has a strong dry season of 6-7 months. We have conducted the censuses with 3-7 day intervals, including mark-recapture of beetles and construction of life tables for up to 9 consecutive years in order to clarify the seasonal change in abundance and mortality of the populations. In most populations, adult number changed largely with the formation of high peaks from time to time at intervals of 6-12 months. Their increase or decrease was gradual, progressing 3-5 months. Even under conditions with sufficient amount of rainfall in Padang, Sukarami and Bogor, oviposition intensity, number of the following immature stages and, as a result, adult emergence frequently showed discrete peaks at a fixed interval. This “generation cycles” were especially clear during the phase of population increase. There was no simple relationship between the seasonality of rainfall and that of the beetle populations. We also discussed the impacts of the strong droughts in 1994 and 1997-1998 caused by El Nino, and the degree of synchronization in the trends of the populations among the adjacent study sites.

References

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Beetle (Coleoptera) Assemblages at Four Different Habitats in Mount Tangkuban Parahu Area, West Java-Indonesia

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Habitat modification has been a common problem these days especially in developing countries such as Indonesia, where habitat modification from natural forest to production forest or to agriculture area is common. Habitat modification can alter species composition and community structure including insect groups. Such modification also occurs in Mount Tangkuban Parahu (MTP) area, one of the natural reserves and active volcanic mountain in West Java, Indonesia.

Coleoptera or beetle is oftern considered as an ecological indicator for habitat modification both in tropical and temperate area. Beetle mostly from Carabidae family has been used as ecological indicator in temperate area; however, it is still difficult to decide the most appropriate group of Beetle that serves as a potential ecological indicator in tropical region [1–4] include in mountainous tropical area such as MTP.

Beetle assemblages at four different habitats of MTP were investigated from April to September 2004. Sampling was carried out at four different types of habitat represented by several dominant types, i.e. Vaccinium forest, mixed forest, pine forest, and post-agricultural area, of plant community. Specimens were collected using four different kinds of traps following sampling methods of DIWPA (Diversitas for Western Pacific Area) for IBOY (International Biodiversity Observation Year) program [5] and analyzed down to the morphospecies level. The results showed that species composition of coleoptera differed at each habitat. Mixed forest was the most diverse with 252 species, followed by pine forest (178 species), Vaccinium forest (90 species) and post-agricultural area (76 species). In addition, many singleton species were found at each sampling site.

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Diversity and Structure of Above-ground Arthropod Assemblages During the Restoration of Satoyama in Kanazawa, Japan

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In Japan, much attention has recently been paid to the importance of “satoyama”, the traditional rural landscapes, in biodiversity conservation. Since 1960s' many satoyama areas in Japan have been destroyed and/or abandoned and left unmanaged resulting in the loss of biodiversity [1]. In the satoyama area surrounding Kanazawa University, many studies have been done on biodiversity, especially insects, and ecological relationships between organisms such as pollination and seed dispersal [2]. Above-ground insects are prevalent in all habitats and variable in ecological guilds, which make them good indicators for quantitative biodiversity evaluation, showing habitat quality [3].

In this study, we analyzed the arthropod samples at higher taxonomic level as a surrogate for biodiversity at the lower taxonomic level (species level). We adopted higher taxonomic level assessment as a rapid procedure to evaluate habitat heterogeneity in satoyama. Above-ground arthropods were collected monthly using window traps from June to November in 2005 and 2006 from ground and upper (5-15m) levels at nine sampling sites in the satoyama area in Kakuma Campus of Kanazawa University, Kanazawa. Out of nine, five sites were in forested areas, while four were in restored areas in a small cultivated valley.

We found that Diptera was the predominant order at upper and ground levels, while other dominant “flying” orders dominated the Window trap samples. Multivariate analysis of faunal composition at order level allowed the distinction of different habitat groups at different levels (strata), and distinguishes the orders into “cultivated valley” and “non-wetland/forest” orders. The “forest” orders were more aggregated compactly among the sites than the “cultivated valley” orders. Low similarity among sites in cultivated valley was detected between years at ground level. Management practices in cultivated valley may be contributed to the changes and preference of some orders in the particular sites.

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Composition and Structure of Litter and Soil Macrofauna Communities in Satoyama Region in Kanazawa, Japan

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The Satoyama system has been proposed as the future Japan Landscape Management that encourages the harmonic interaction between human and its environment. This system with its mosaic habitat is believed to be able to conserving the biodiversity in the term of species richness and ecological processes.
Within a heterogeneous land-use system, like Satoyama, the different plant species and soil management may lead to different living condition to litter and soil fauna. This fauna are important to many ecosystem processes, such as decomposition, nutrient cycling, and maintaining biological, chemical, and physical character of the soil ecosystem [1,2].

We surveyed the soil macrofauna species composition on a Satoyama Region in Kitadan Valley and Kakuma Forest (South East of Kanazawa City, Ishikawa, Japan). The Kakuma Forest mainly consisted of deciduous broad leaved trees which were predominated by two oak species, *Quercus serrata* and *Q. variabilis* and patches of plantations of Japanese cedar (sugi) *Cryptomeria japonica* and moso bamboo *Phyllostachys* sp. Terraced paddies in Kitadan, a small valley (0.5 ha) have been restored gradually by local volunteers for nature education and biodiversity research since 2002.

Arthropod was the most abundance macrofauna, with Formicidae as major taxa, found in study site. All sampling site that represented the habitat mosaics in Satoyama system showed no differences on total number of soil and litter fauna among them. However, some taxas showed preference to certain habitat type and can be divided into several distinctive groups with specific environmental condition.

From all four physical factors observed, only soil temperature had the influence to soil and litter macrofauna. Even thought not strongly effect the distribution and composition of soil and litter macrofauna, amount litter and humidity provide a limiting factor for Isopoda and Tubificida. On the other hand traditional paddy cultivation might provide benefit for some important soil decomposer like earthworm.

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Changes of Local Pollination Ecology during Restoration of Satoyama System

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Human have changed almost all earth landscape for fulfilling their need in natural resources. Increase in the human needs accelerate the rate of change by great amount which caused problems with environment and all the life systems in it. Realizing this condition, recently the effort to restore the degraded environment has been attracted more attention worldwide. Among all the methods to restore previous condition is using the traditional landscape management.

Before the industrialization of agriculture, Japan had developed a unique landscape management called Satoyama. Satoyama itself is a buffer zone between the wild forests and the settled communities. This established an area where people lived in intimate contact with nature. In this system bamboo forests, secondary forests, and small patches of grassland created an integrated landscape with plantations, irrigated ponds, irrigation channels, and agriculture area [1]. The environmental patchiness of this system provide many beneficial functions not only for human but also to plants and animals inside it as have been investigated by some groups [2,3].

The benefit of this system not only to plants and animals inside it but also the life system that produced by the interaction of both. In order to assess the benefit and progress of restoration, we used pollination system as our study subject. Pollination by animals is ubiquitous in terrestrial habitat involving about 67% of flowering plant species and involving a high diversity of insect species. Thus, this type of plant-animal relationship may also act as a good bio-indicator for the successful of habitat management as suggested by other groups who work on other restoration project [4]. The study was conducted in small valley inside of Kanazawa University Satoyama system, called Kitadan Valley, which a 30-years old abandoned Satoyama paddy field. The restoration work was started at 2003 by reinstate the traditional paddy cultivation

In this talk, we present our result on the investigation of pollination system during our four years study. We discuss the seasonal changes of abundance and richness in flower visiting insects and its visited flower species during restoration. From the data of richness and abundance of flower visiting insects we discuss the diversity and evenness of each insect orders in relation to the stability of community. Finally, we discuss the changes of flower preference and its relation with the changes in abundance of some dominant flower visiting insects.

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Heavy oil spill accidents in Japan, Korea and Indonesia:

International joint project between Kanazawa University and Bandung Institute Technology

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The oil spill accident occurred when a Hong Kong-registered supertanker (Hebei Spirit) was rammed by a South Korean-owned barge that came unmoored from its tugboat in rough seas about 10 km off Mallipo Beach at Taean Peninsula, South Korea. The 3 kinds of oil spill accidents started at 7:00 on December 7th, 2007, when a tanker collided with a barge, and blackened once-scenic beach along South Korea's western coast, about 150km, southwest of Seoul. A total of 12,547 kl of both heavy oil and crude oil gushed into the ocean, more than twice as much as in South Korea's previous worst spill, in 1995. Local residents worked with about 8,800 peoples of volunteers, civil servants, police officers and military personnel, were engaged in the effort to clear away oil on the region's shores. The seafood, oyster farms and tourism industries in the Taean region have been devastated. Oil blanketed the sand of Mallipo Beach and the rocks of Euhang Beach at Taean Peninsula, South Korea, were studied on January 5-6th 2008, just after one month of the accident. Residents wore overalls, used shovels, buckets, adsorption mats, tatters, oil fences, hand-made adsorption roller, heated water at 50-70 □ washing bath, and high-pressured nozzle to clean up the oil muck. The purification of oil on the sand beach was made so quickly within one month in sandy Mallipo Beach, whereas abundant oil drops between rocks with oil slick on the seawater surface on the rocky beach in Euhang Beach still remain. The oil-contaminated hazard map by Marine Environmental Risk Assessment Research Division, Korea Ocean Research and Development Institute, Korea, reported on December 18-19th, 2007. In this study, on-site surveys for checking and observing the oiling condition have started on January 5-6th 2008 one month after the spill at Mallipo Beach and Euhang Beach. Compared with common natural seawater (pH 8.2-8.3; EC 37.5-45.5 mS/cm) of the Sea of Japan (East Sea), the values of pH and EC in two places indicated that the bioremediation process of oil took place under neutral conditions (pH 7.2-7.4; EC 26.1-43.9 mS/cm). The analytical data of volatile aromatic hydrocarbon concentrations for 0.5 ?/min at two beaches indicated that the concentration of toluene is quite higher in the atmosphere than that of C typed heavy oil from the Nakhodka tanker in January 1997 in Japan. Because the origin of oils is different between crude oil and heavy oil. The both of oils in Korea and Japan accidents contain high S element associated with Si characteristics.we must find new defensive measure systems which are safe, low cost, easy, and sustainable by using local natural materials, such as soils and clays.

The Research Road Map of Physics of Electronics and Materials, Research Group of ITB

Sukirno

The Physics of Electronics and Materials

Abstract

The research Road Map of Physics of Electronics and Materials consists of Functional Materials and Functional Devices. The first is divided into amorphous materials, μ/poly/single crystalline materials, nano-materials (included nano-particle and nano-catalyst), higk K materials, III-V compound semiconductors, Diluted Magnetic Semiconductor as well as oxide and superconductor materials. The second is divided into the following: Amorphous Solar Cell, Sensor and Photodetector, FET, MOSFET/HEMT/TFT, TEFLED/Laser Diode, Fuel Cells and Single Electron Devices.

In our Research Group, we have at least 4 (four) reactor systems i.e: PECVD (Plasma Enhanced Chemical Vapor Deposition), MOCVD (Metal-Organic CVD), PVD (Physical Vapor Deposition which includes PLAD (Pulse Laser Assisted Deposition) and Un-balanced Magnetron Sputtering System) as well as Photo-CVD.

In term of theoretical and simulation aspects, we also conduct the research on electronic scattering, distribution of electronic and hole carriers for carbon materials, mechanism of tunneling current, simulation of electronic and opto-electronic devices as well as simulation for mechanism of fluid dynamics in the reactor chambers.

In this presentation, we will present the current topics of our group on calculation and simulation results on mechanism of fluid dynamics in the reactor chambers and also on electronic scattering, distribution of electronic and hole carriers for carbon materials, mechanism of tunneling current, simulation of electronic and opto-electronic devices.

First-principles molecular dynamics method with noncollinear magnetism

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In our progresses, noncollinear magnetism has been available for simulating a magnetic system with using an idea based on the Car-Parrinello molecular dynamics [1,2]. The new scheme was developed in a pseudopotential plane wave method, associated with two-component spinor wave functions. In this method, the direction of the magnetization is a continuous variable of position. It allows us to relax the atomic and magnetic structures simultaneously and self-consistently. I will address an application to small Fe clusters and their oxide ones and then, an application to a system of liquid oxygen [3,4]. In the latter, performing the molecular dynamics, both magnetic and structural correlation could be observed simultaneously, as well as the atomic structure factor and the magnetic structure factor were found to agree well with those of experimental counterparts.

The noncollinear scheme with two-component spinor easily allows us to introduce spin-orbit interaction (SOI) in our simulation code. The SOI which results from relativistic effects is important for materials having heavy elements. We have developed ultrasoft pseudopotentials (USPPs) which include fully relativistic effects and applied them, first of all, to some fcc bulks and then, the magnetic materials which has a large magnetic anisotropy [5].

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Development of fully relativistic pseudopotentials and application to the sixth-row elements of the periodic table

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In the system having heavy element or magnetic one, relativistic effects on electron motion are important for material properties. We have developed a ultrasoft pseudopotential (USPP) which includes fully relativistic effects. In the generation process, a Dirac-type equation is solved instead of a Schrodinger-type equation. This USPP involves spin-orbit interaction (SOI) and is combined with the formalism of two-component-spinor wavefunctions [1] within Kohn-Sham theory.

In the previous works [2,3], we performed a transferability test for isolated atoms and obtained an equilibrium lattice constant for the fcc metallic bulks. These results were in good agreement with experimental one. For the magnetic bulk of FePt, our approach nicely described the property of magnetic anisotropy, compared with the all electron approach.

In the present work, we show the quilibrium lattice constant, bulk modulus, band structure, for the elements from $_{72}$Hf to $_{82}$Pb. We performed the fully-relativistic calculation(FR) which included SOI by using the USPP we developed and the scalar-relativistic calculation(SR) which didn't include SOI. We used LDA(Ceperley-Alder-Perdew-Zunger) to exchange-correlation energy. The equilibrium lattice constant obtained is at most 2% smaller than experimental value, and is corresponding well for all elements. For the property of bulk modulus, FR mostly tends to provide a better agreement with the experimental value than SR. But both of them don't so reproduce the experimental value especially for the element which has the large atomic number. The maximum difference with experiment is found to be 16% for Au in FR cases. We investigated effects of SOI by comparing FR and SR. Whereas the SOI doesn't affect lattice constant and bulk modulus so much, it causes some visible spin-orbit splittings in band structures.

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Electronic structures and magnetic anisotropies of thin iron films on platinum surfaces

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FePt and CoPt alloys are a promising magnetic material for ultra high density recording media due to their large perpendicular magnetic anisotropy energy (MAE). Gambardella *et al*. fabricated a Co nano-wire on Pt surface by using a self-assembly epitaxial technique and characterized magnetic properties of the system[1]. The similar system, thin Fe layer on the Pt surfaces, has been studied by Repetto *et al*. [2]. It is interesting to investigate the magnetic properties of thin filmes and nanostructures on the metallic surfaces.

We have studied magnetic anisotropies of Fe atoms on the Pt(111) and Pt(001) surfaces, employing local spin density approximation in the Kohn-Sham theory. We used the pseudopotential planewave method with the fully relativistic version in which the wavefunction has the two-component spinor form [3]. This method contains self-consistently the spin-orbit coupling, which is the main origin of magnetic anisotropy. We calculated MAE, magnetic moment and local density of state (LDOS). We also investigated the effect of surface relaxation for the magnetic anisotropy.

In Pt (111) surface, we investigated the three coverages for Fe monolayer: the full coverage, the half coverage and the quarter coverage. For the half coverage, Fe atoms were assumed to form chains along a [1$\bar{1}$0] direction. For all cases, it was found that the magnetic easy axis of system is within the surface plane. In case of the half coverage, the magnetic easy axis is directed to the alignment of Fe atoms.

We investigated Pt(001) surface covered with Fe monolayer. The MAE was very small in this system, as shown in Fig. 1. But this system has get a large perpendicular magnetic anisotropy (MAE=5.23meV/Fe atom) with a combination of Pt overlayer[4].

We will addresse the relationship between surface local structure and magnetic anisotropy from the LDOS and the band dispersion.

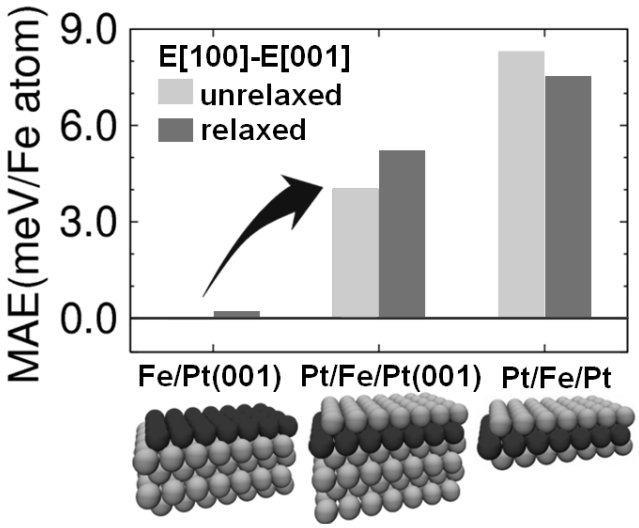

Fig.1:Pt(001) surface models and MAEs.

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Instabilities of Steps on a Vicinal Face

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When temperature is lower than the roughing temperature, crystal surface is covered with steps and terraces. The surface, which consists of straight parallel steps, is called a vicinal face (Figure 1 (a)). On the vicinal face, the steps show two types of instabilities. One is step wandering, which is the instability against the fluctuation along the step, and the other is bunching, which is the instability against fluctuation of the step distance and the other is step.

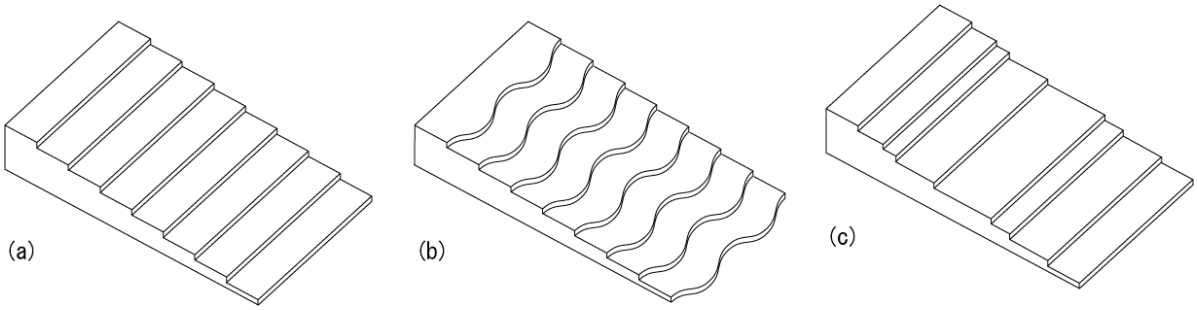

Figure 1 Step instabilities on (a) vicinal face: (b) step wandering and (c) step bunching.

On the Si(001) surfaces, the step instabilities occur when the crystal is heated by the direct electric current. The cause of the instabilities is the drift flow of adatoms [1], which is caused by the direct electric current. On the vicinal face, the dimerization of surface atoms occurs and the surface diffusion of adatoms are anistropic. With taking account of the anisotropy, we study the step instabilities induced by the drift of adatoms. We use a simplified model and carry out Monte Carlo simulation [2]. The step bunching occurs irrespective of the drift direction, but the form of bunches changes with the drift direction: the fluctuation of bunches with step-up drift is larger than that with step-down drift, which agree with the experiments [3].

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Chemical Processes in the Superfluid Helium

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Recent progresses in experimental techniques have made it possible to implant guest atoms and molecules in helium nano-droplets. The new experimental methods have opened up a new interdisciplinary branch of spectroscopic research with interesting applications [1]. An impressive example is provided by oxygen carbon sulfide (OCS) molecules dissolved in the helium droplets. The infrared spectrum of the OCS molecules at temperature 0.37 K indicates that the molecules rotate freely in the condensed medium. The helium-4 droplets at the temperature are expected to be in a superfluid state characterized by nearly zero "viscosity"; thus, the above-mentioned free-rotor behavior can be attributed to the superfluidity at a molecular level. In the present study, a single OCS molecule in small helium-4 clusters has been studied using path integral simulation techniques to address this issue theoretically. Helium atoms as a bosonic many-body system are handled by our path integral hybrid Monte Carlo method [2]. Rotational degree of freedom of the molecule is incorporated in the hybrid Monte Carlo using a newly developed "Legendre potential" technique [3,4]. In my talk, selected results on the OCS-doped helium clusters [2-5] will be presented.

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Reviews on the quantum control of molecular system by laser field

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Due to the great development of laser technique, several optical methods have been introduced to control the chemical reaction using the laser pulses in the picosecond time domain. In this talk, we briefly explain several laser control theories and review our related works.

Tannor and Rice have presented the pump–dump scheme, where the pump pulse first creates the wavepacket on the excited potential energy surface, and after an appropriate time delay, the dump pulse induces the stimulated transition to the desired state. The π -pulse method being familiar in the recent FTNMR is also applied to induce the population inversion of molecule in the optical experiment. The basic principle is very simple, but in order to experimentally achieve the complete transition, the pulse shape has to satisfy the strict condition. Rabitz et al. have proposed an optimal control theory, which make theoretically a highly effective pulse, but the resultant pulse shape is usually very complex to be made experimentally.

Bergmann et al. proposed the stimulated Raman adiabatic passage (STIRAP) to realize the complete population transfer between vibrational levels. The STIRAP method has a counterintuitive pulse sequence, a rather large overlap between two pulses, and a larger pulse width compared to the π -pulse width. This method has some advantages on the formation of the pulse shape. Namely, it has very flexible conditions for the laser parameters such as amplitude, frequency, or pulse width, and is well known as very effective method for population transfer in three level systems.

Due to the robustness with respect to the laser parameters, therefore we applied the STIRAP to control the proton motion of 1-methylmalonaldehyde, and found out the effective pulse sequence to yield the complete proton transfer, applying the one-dimensional asymmetric double well potential. This method is also applied to the control of the isomerization reaction and the state-selective electronic excitation of diatomic molecules. Recently, we have been investigating the multiphoton processes involving the continuum state, such as photodissociation and photoassociation.

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Measuring Disordered degree in Shape Fluctuation of Few Correlated Phospholipids

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Body of abstract

Biological phospholipids have important functions in biological systems. In this talk, we discuss their dynamics for few correlated phospholipids. Since they have irregular shapes, we pay attention to measure degree of disordered for such kind of systems. We simulate some phospholipids by using Molecular Dynamics simulation. To evaluate their fluctuation, we calculate by using our previous methods based on concept of Aperture, Symmetry, Isotropy, and Compactness dynamics. We analyze disordered degree for their transition among certain geometrical pattern. In addition, we discuss cooperative phenomena in connection their frequency for the possibility of strong or soft mode and transition phenomena. Furthermore, we also discuss the fluctuation line in connection with non-Gaussian distribution.

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Brownian dynamics simulation of polyimide gel

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Gels are useful materials because of its network structure. Furukawa and coworkers have performed scanning microscopic light-scattering (SMILS) experiments [1] and obtained the distribution of network size of gels.

We studied the formation process and the structure of gels by simulation for the polyimide gels. Our model is based on the gels used in the experiments of He et al., [2] where oligomers with different flexibility were used. Hosono et al have analysed photoresponsive jungle-gym-type gels [3] .

In our model, we use the triangular unit designating a trifunctional crosslinker, and the linear unit designating oligomer as main chain. We perform Brownian dynamics simulation [4] using the following Langevin equation:

$$m_i \frac{d^2\mathbf{r}_i}{dt^2} = -\frac{\partial U}{\partial \mathbf{r}_i} - \zeta \frac{d\mathbf{r}_i}{dt} + \mathbf{g}_i(t) \qquad (1)$$

The second term of the right hand side is the effect of the viscosity, and the third term is the random force caused by solvent molecules.

In Fig.1, the snapshots of the maximum clusters in each system are shown. For the rigid model, gel forms extending structure; for the flexible model, gel forms shrinking structure. We can observe that heterogeneity is enhanced by flexibility. We analysed the growth of clusters and the loop structure. Other results will be reported in the talk.

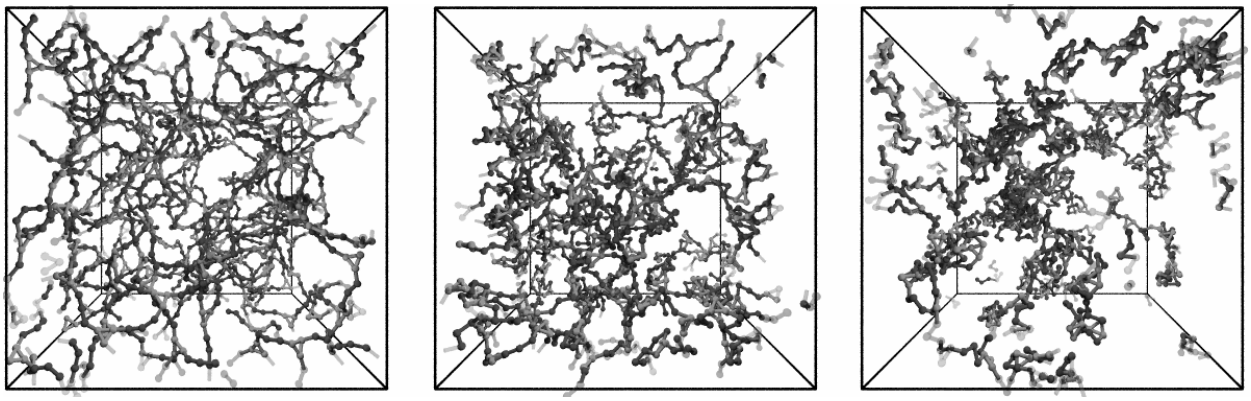

Fig 1 Snapshots of simulations. (a) for rigid main chain model, (b) for semi-rigid main chain model and (c) for flexible main chain model.

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Ab initio Quantum Chemical Study of the Thermal Decomposition of Aromatic Substituted *N*-acylhydrazones and *N*-thioacylhydrazones

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An *ab initio* quantum chemical study of the initial steps of the thermal decomposition of *N*-acylhydrazones and *N*-thioacylhydrazones is reported. Using G2(MP2) methods, the thermochemistry and rate parameters of a number of key reactions have been obtained, and the effects of several substituents have been revealed. The crucial step in each is the tautomerization via an open six-membered ring and concurrently accompanied by the N-N bond fission of the hydrazones. The calculated critical energies of the reactions are consistent with the experimental activation energies previously obtained by Al-Awadi, et. al. in 2006.

Spectral Simulation of Carbon Allotropes

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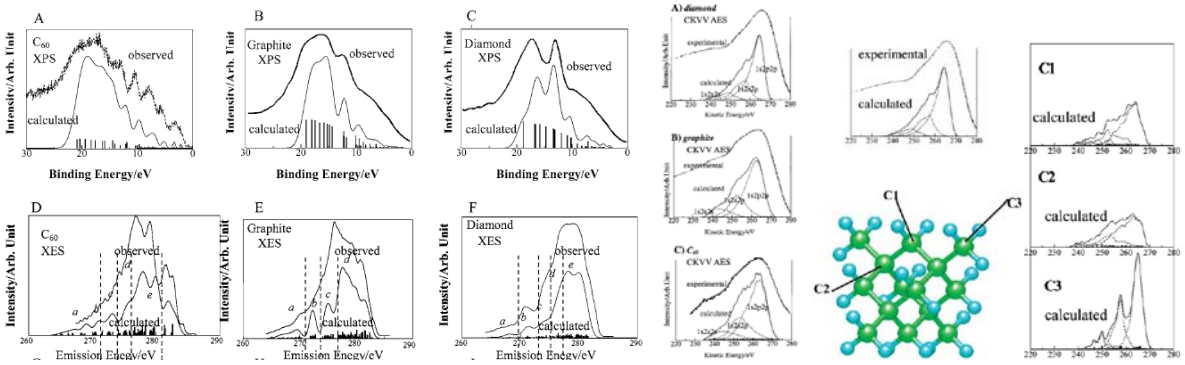
Simulation of electron spectra (valence XPS, C Kα XES, and AES) for carbon allotropes was performed by DFT methods using the model molecules in the three following cases.

In the 1st case, combination analysis of the valence XPS, C Kα XES, and AES for the allotropes (diamond, graphite and fullerene) is demonstrated by deMon DFT calculations using the model adamantane derivative ($C_{10}H_{12}(CH_3)_4$), pyrene ($C_{16}H_{10}$) and C_{60} molecules, respectively [1]. The theoretical valence photoelectron, C Kα X-ray emission, and auger electron spectra for the allotropes are in good accordance with the experimental ones. The experimental Auger electron spectra of the allotropes can be classified in each range of 1s-2p2p, 1s-2s2p, and 1s-2s2s transitions for C-KVV spectra, and in individual contributions of the chemically different carbon atoms from theoretical analysis.



In the 2nd and 3rd cases, we performed DFT calculations using Amsterdam density functional (ADF) program to simulate X-ray photoelectron spectra for carbon allotropes (diamond, graphite, single-wall carbon nanotube (SWCN), and fullerene C_{60}). We firstly described the simulation method for valence electron spectra to distinguish the diamond phase of carbon from the graphite carbon, and secondly evaluated the WD values from the differences between the calculated core-electron binding energies (CEBE)s of the model molecules (using ΔE_{KS} approach (like ΔSCF method in MO)) and experimental CEBEs of carbon allotropes. The WD values of carbon allotropes correspond to the order of experimental values (CNT < graphite < diamond < C_{60}) for work functions obtained from accurate cylindrical analyzer (CMA) detector by Goto's and co-workers.

Table 1. CEBEs, WD, and work function for carbon allotropes

Carbon	**Core-electron binding energy (eV)**		WD	work function(obsd)*	
Allotropes	Calc.(model)	Exp.		**as evacuated**	**after Ar ion sputtering**
Diamond	**290.01-290.26**	**284.4**	**5.61-5.86**	**4.83**	**4.38→4.51**
Graphite	**289.67-290.14**	**284.3**	**5.37-5.84**	**4.73**	**4.37→4.63**
CNT	**289.65-289.85**	**284.55**	**5.10-5.30**	**4.35-4.77**	**4.20→4.40**
C_{60}	**290.46**	**284.7**	**5.76**	**6.16**	**5.65→6.12**

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Theoretical Auger spectra of molecule by two-electron propagator method

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Double ionization potential (DIP) which is defined as energy required for detachment of two electrons from a neutral molecule, has been studied extensively using a variety of experimental techniques. Auger electron spectroscopy has been the most widely used method to investigate the double ionized state of molecule. In theoretical investigation of the double ionization process, the electronic energy difference method based on configuration interaction (ΔCI) may be one of the most accurate methods. ΔCI calculations, however, cannot be carried out for most system of chemical interest because a very large matrix eigenvalue problem must be solved even for small molecule.

On the other hand, an electron propagator theory underlies many methods for calculating single electron binding and excitation energies[1]. The accuracy and computational efficiency have been realized through use of recently derived approximations for vertical single electron detachment energies[2]. Additionally electron propagator method can be determined the whole spectra all at once in a single calculation in contrast to the ΔCI calculation. Therefore some approximations to the exact two-electron (two-particle or particle-particle) propagator which obey the Dyson or the Bethe-Salpeter equation have been developed and used to study the double ionization process.

In this study, the second order two-electron Dyson propagator is derived in the superoperator theory. Numerical results of the DIPs for H_2O, C_2H_4 and H_2CO molecules by this method are compared to results with the conventional ΔCISD, the other propagator method and the experimental values. Theoretical Auger electron spectra of the three molecules are simulated with the intensities computed by the 2-hole analysis, for example as shown in Figure for the water molecule. Finally we will discuss advantages on the DIPs calculation and the Auger electron spectral simulation by the new propagator method.

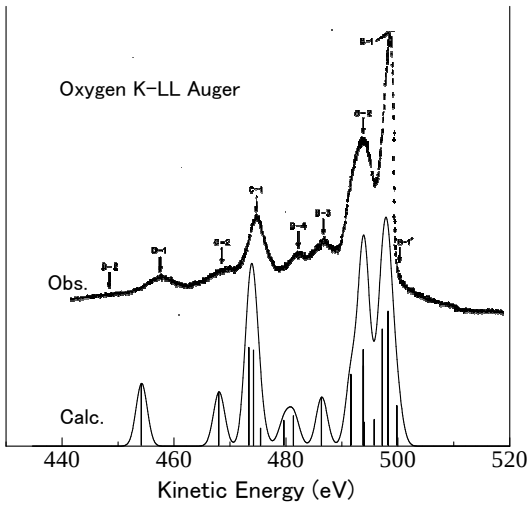

Figure. Theoretical oxygen K–LL Auger electron spectrum of water molecule with the experimental one.

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