THE 12th ASIA COMPUTATIONAL MATERIALS DESIGN WORKSHOP

Binh Duong-Vietnam, 14th-16th April 2022

12th ASIA COMPUTATIONAL MATERIALS DESIGN WORKSHOP 2022 (ACMD 2022, Vietnam)

With the aim of imparting modern quantum simulation techniques, the Asia Computational Materials Design Workshop (ACMD) co-organized by Osaka University-Japan and universities of Vietnam has been held in Vietnam since 2009 many times. In 2022, ACMD will be held at Thu Dau Mot University-Vietnam. This workshop will provide lectures on cutting-edge research in computational materials design as well as hands-on lectures in quantum simulation. The workshop will also include lectures with an overview of the role of CMD in Vietnam, computational techniques for electronic structures, and applications in designing new functional materials. Furthermore, some of the original quantum simulation packages developed by professors of Osaka University will be introduced by the developers in hands-on lectures on the high-performance computing system of Thu Dau Mot University (TDMU HPCC).

Với mục đích truyền đạt các kỹ thuật mô phỏng lượng tử hiện đại, Hội thảo về thiết kế các vật liệu tính toán (CMD) Châu Á (ACMD) đã được tổ chức tại Việt Nam từ năm 2009 với sự hợp tác của Đại học Osaka và các trường đại học tại Việt Nam trong nhiều lần. Năm 2022, ACMD sẽ được tổ chức tại Đại học Thủ Dầu Một. Hội thảo này sẽ cung cấp các bài giảng về các nghiên cứu tiên tiến trong thiết kế vật liệu tính toán cũng như đào tạo thực hành về mô phỏng lượng tử. Hội thảo cũng sẽ bao gồm các bài giảng với tổng quan về vai trò của CMD tại Việt Nam, các kỹ thuật tính toán cấu trúc điện tử cùng với các ứng dụng của chúng để thiết kế các vật liệu chức năng mới. Hơn nữa, một số gói mô phỏng lượng tử

guyên lý ban đầu được phát triển bởi các giáo sư của trường Đại học Osaka sẽ được các giáo sư giới thiệu trong các khóa đào tạo thực hành trên hệ thống tính toán hiệu năng cao của trường Đại học Thủ Dầu Một (TDMU HPCC).

現代の量子シミュレーション技術を提供することを目的として、大阪大学-日本とベトナムの大学が共催するアジア計算材料設計ワークショップ（ACMD）が 2009 年から何度もベトナムで開催されています。2022 年、ACMD はベトナムのトゥーダウモト大学で開催されます。このワークショップでは、計算材料設計の最先端研究と量子シミュレーションの実地講義を行います。このワークショップには、ベトナムにおける CMD の役割の概要、電子構造の計算技術、および新しい機能性材料の設計への応用に関する講義も含まれます。さらに、大阪大学の教授によって開発されたオリジナルの量子シミュレーションパッケージのいくつかは、トゥーダウモト大学（TDMU HPCC）の高性能コンピューティングシステムに関する実践的な講義で開発者によって紹介されます。

International Organizers

Assoc. Prof. Nguyen Van Hiep, Chairman of the Board, Thu Dau Mot University, Vietnam;

Prof. Yoshitada Morikawa, Graduate School of Engineering, Osaka University, Japan;

Prof. Tamio Oguchi, Center for Spintronics Research Network, Osaka University, Japan;

Prof. Dinh Van An, Graduate School of Engineering, Osaka University, Japan.

Local Organizers

Assoc. Prof. Vo Van On, Institute of Applied Technology, Thu Dau Mot University, Vietnam;

Assoc. Prof. Nguyen Thanh Tien, College of Sciences, Can Tho University, Vietnam;

Dr. Nguyen Duy Khanh, Information Technology Center, Thu Dau Mot University, Vietnam.

Lecturers

Prof. Yoshitada Morikawa, Graduate School of Engineering, Osaka University, Japan;

Prof. Tamio Oguchi, Center for Spintronics Research Network, Osaka University, Japan;

Prof. Nguyen The Toan, Hanoi University of Science (VNU-HUS);

Assoc. Prof. Sato Kazunori, Graduate School of Engineering, Osaka University, Japan;

Assoc. Prof. Wilson Agerico Diño, Graduate School of Engineering, Osaka University, Japan;

Assoc. Prof. Ikutaro Hamada, Graduate School of Engineering, Osaka University, Japan

Assoc. Prof. Nguyen Thanh Tien, College of Natural Sciences, Can Tho University, Vietnam;

Assoc. Prof. Do Ngoc Son, Faculty of Applied Science, HCM University of Technology, Vietnam;

Dr. Nguyen Duy Khanh, Information Technology Center, Thu Dau Mot University, Vietnam.

Secretaries

Dr. Nguyen Duy Khanh, Information Technology Center, Thu Dau Mot University, Vietnam;

Mr. Huynh Than Phuc, Information Technology Center, Thu Dau Mot University, Vietnam.

WORKSHOP PROGRAM

ACMD 2022

Guest Room 1 (**VIP 1**), HPCC Room (**HPC.R**), Thu Dau Mot University

14 April	15 April	16 April
07:30-08:00: **VIP 1** **Registration**	Chair: Dr. Duy Khanh NGUYEN, Thu Dau Mot University	Chair: Assoc. Prof. Vo Van On, Thu Dau Mot University
08:00-08:25, **VIP 1** **Opening remarks** Assoc. Prof. Nguyen Van Hiep, Thu Dau Mot University Prof. Yoshitada Morikawa, Osaka University 08:25-08:30: **VIP 1** **Group Picture** Chair: Assoc. Prof. Vo Van On, Thu Dau Mot University 08:30-9:30: **VIP 1** **Brief Tutorial on Basic Linux and HPCC connection** Dr. Nguyen Duy Khanh, Thu Dau Mot University ***Break (10 mins)*** 9:40-10:40: **VIP 1** **Basic Theory for AkaiKKR** Assoc. Prof. Sato Kazunori, Osaka University 10:40-11:40, **HPC.R** **Hands-on Tutorial 1 (AkaiKKR)**	08:30-09:30, **VIP 1** **Basic Theory for HiLAPW** Prof. Tamio Oguchi, Osaka University ***Break (10 mins)*** 9:40 – 11:40: **HPC.R** **Hands-on Tutorial 2 (HiLAPW)** Prof. Tamio Oguchi, Osaka University	08:30-09:30, **VIP 1** **Basic Theory for STATE-Senri** Prof. Yoshitada Morikawa, Osaka University ***Break (10 mins)*** 9:40 – 11:40: **VIP 1** **Hands-on Tutorial 3 (STATE-Senri)** Assoc. Prof. Ikutaro Hamada and Prof. Yoshitada Morikawa, Osaka University

Assoc. Prof. Sato Kazunori, Osaka University		
Lunch (1h20 mins)	**Lunch (1h20 mins)**	**Lunch (1h20 mins)**
13:00-15:00, **HPC.R Hands-on Tutorial 1 (AkaiKKR)** Assoc. Prof. Sato Kazunori, Osaka University ***Break (10 mins)***	13:00-15:00, **HPC.R** **Hands-on Tutorial 2 (HiLAPW)** Prof. Tamio Oguchi, Osaka University ***Break (10 mins)***	13:00-15:00, **HPC.R** **Hands-on Tutorial 3** (STATE-Senri) Assoc. Prof. Ikutaro Hamada and Prof. Yoshitada Morikawa, Osaka University ***Break (10 mins)***
Chair: Assoc. Prof. Vo Van On, Thu Dau Mot University 15:10-15:50, **VIP 1** **Special Lecture 1** Magnetoresistance within Boltzmann theory Prof. Tamio Oguchi, Osaka University 15:50- 16:30, **VIP 1** **Special Lecture 2** van der Waals density functional applied to surfaces and interfaces Assoc. Prof. Ikutaro Hamada, Osaka University 16:30- 17:10, **VIP 1** **Special Lecture 3** Structural, electronic, and optical properties of defective sawtooth penta-graphene nanoribbons: An DFT insight Assoc. Prof. Nguyen Thanh Tien, Can Tho University	Chair: Assoc. Prof. Nguyen Thanh Tien, Can Tho University 15:10- 15:50, **VIP 1** **Special Lecture 4** Surface as a playground for exploring physical phenomena and a foundation for realizing designer materials: Some hydrogen-surface reaction related case studies Assoc. Prof. Wilson Agerico Diño, Osaka University 15:50- 16:30, **VIP 1** **Special Lecture 5** Theoretical study of hydrogenation process of CO_2 on metal catalysts Prof. Yoshitada Morikawa, Osaka University 16:30- 17:10, **VIP 1** **Special Lecture 6** Understanding molecular mechanism of alluporinol SCAR reaction in Vietnamese patient using computer simulation Prof. Nguyen The Toan, Hanoi University of Science (VNU-HUS)	Chair: Prof. Dinh Van An, Osaka University 15:10-15:50, **VIP 1** **Special Lecture 7** First-principles study of electronic and optical properties of Au/LaAlO3/SrTiO3 heterointerface Assoc. Prof. Do Ngoc Son, HCM University of Technology 15:50-16:30: **VIP 1** **Special Lecture 8** In silico studies of monolayer systems Dr. Nguyen Duy Khanh, Thu Dau Mot University 16:30–16:40: **VIP 1** **Certification Conferring and Closing Remarks** Prof. Yoshitada Morikawa, Osaka University Assoc. Prof. Vo Van On, Thu Dau Mot University

OUTLINE

Introduction to GNU/Linux in High-Performance Computing Architecture

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Abstract

Currently, the top 500 supercomputers in the world is fully based on GNU/Linux OS. Besides, most of the servers powering the Internet and high-performace computing clusters (HPCC) are also based on Linux. This means that the understanding of Linux structures is very essential to operate supercomputers or HPCC. In this talk, I will present various topics related to Linux in HPCC that can fully provide how to operate tasks in HPCC. The topics include the background and history, the command line, directory structure, files, text display and search, users and permissions, processes, the vim and vi text editors, shell scripting, system configuration files, SSH connections, SSH graphics and file transfer. Besides, the brief introduction to high-performance computing cluster of Thu Dau Mot University (TDMU HPCC) and how to operate TDMU HPCC for hands-on tutorials at the ACMD 2022 will be also presented.

Keywords: Unix, GNU/Linux, server, high-performance computing cluster, command lines, and linux distributions.

Basic Theory for AkaiKKR

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Abstract

In this document, how to use Machikaneyama2002 (AkaiKKR), a KKR-CPA-LDA package, is briefly guided. The KKR method is one of the methods of electronic structure calculation and is also called "Green's function method." KKR indicates the initials of Korringa, Kohn, and Rostoker, who invented this method. CPA means the coherent potential approximation, which can deal with random systems. Green's function might be difficult to understand if you are trained with ordinary band structure calculations, which solve an eigenvalue problem by diagonalization. However, you can apply KKR-CPA to much wider range of situation than ordinary band structure calculations can do. For example, it can deal with finite temperature magnetism and partial disorder systems since CPA can treat not only periodic systems but also random systems.

Magnetoresistance within Boltzmann Theory

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Abstract

In metals, additional terms in resistivity tensor usually appear depending on a magnetic field B, known as the magnetoresistance (MR) effect due to Lorentz force acting on electrons. Within the Boltzmann theory, the conductivity tensor, which is the inverse matrix of resistivity, can be written using the group velocity of electrons and relaxation time assumed [1-3]. Up to the first order of B, MR is mainly about the Hall effect computed with the group velocity at the Fermi energy (the so-called Fermi velocity) and its derivatives [3-7]. In general orders of B, the equation of motion for electrons in *k* space is solved for a given B and the group velocity is averaged out on the Lorentz orbits perpendicular to B over past relaxation time to obtain the distribution function and resultant conductivity tensor [2]. Therefore, it is concluded that the MR effect becomes significant beyond the simple Hall regime unless the variation of the Fermi velocity is negligible in a *k*-space range of the velocity times relaxation time. A code to compute MR as a post process of band structure calculations was developed and examined for several representative cases such as alkali metals, Cu, and Bi [8].

References:

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van der Waals Density Functional Applied to Surfaces and Interfaces

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Abstract

The dispersion or the van der Waals force is one the most fundamental intermolecular interactions, but is notoriously difficult to describe in density functional theory calculations within the local density and generalized gradient approximations. The nonlocal van der Waals density functional [1] is a class of the exchange-correlation functional that is able to describe the dispersion forces on the same footing as the covalent bonding in a seamless fashion. In this talk, I give a brief introduction to the van der Waals density functional and its implementation [2], with some applications relevant to the surface and interface problems [3].

References:

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Structural, Electronic, and Optical Properties of Defective Sawtooth Penta-Graphene Nanoribbons: An DFT Insight

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Abstract

Pentagon-based 2D materials are receiving increasing attention because of their unique atomic configurations, rich physical and chemical properties, and their promise for broad applications. In 2015, based on extensive theoretical simulations, a group of scientists proposed a 2D carbon allotrope composed entirely of pentagons, penta-graphene, which has a 2D projection resembling the famous 2D pattern named Cairo pentagon tiling. Although penta-graphene is metastable thermodynamically compared to graphene, it is dynamically and mechanically stable, and can withstand high temperatures up to 1000 K. The thermodynamic stability of penta-graphene over the synthesized smallest fullerene C20 implies that it could be realized experimentally. Due to the exotic atomic configuration, penta-graphene exhibits an array of intriguing properties, such as negative Poisson's ratio and ultrahigh ideal strength that can even outperform graphene. Penta-graphene and its derivatives exhibit great potential for applications in nanoelectronics and nanomechanics.

In this lecture, we present first-principles calculations of the structural, electronic, transport, and optical properties of defective sawtooth penta-graphene nanoribbons (D-SSPGNRs). The calculated results of the binding energy and phonon band structure show that the single- and double-vacancy SSPGNR structures with four various chain widths may stabilize with different topologies in the vacancies. Electronic structure calculations denote that the semiconducting D-SSPGNRs appear confined electronic states in the band gap. The electronic transmission spectrum through the D-SSPGNRs is attenuated. Optical properties are investigated by calculating complex dielectric function and optical absorption coefficient with different polarization directions. The imaginary parts of the dielectric function and the absorption coefficient of D-SSPGNR structures expose the new peaks and redshift. Optical polarization occurs in all structures and occurs strongly with the SSPGNRs which are vacated at the sp-hybrid carbon atom.

Keywords: First-principles calculations; Pentagon-based nanoribbons; Electronic Properties; Optical Properties; Optoelectronic device.

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Surface as a Playground for Exploring Physical Phenomena and a Foundation for Realizing Designer Materials: Some Hydrogen-Surface Reaction Related Case Studies

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Abstract

"*... He who controls the spice controls the Universe ...*," declared Baron Harkonnen in the 1984 film adaptation of Frank Herbert's 1965 novel ***Dune*** [1]. But, what is "*the spice*"? It can *extend youth... prolong life... increase vitality... heighten awareness... catalyze interstellar travel... use to make paper... plastics... cloths... fibers...* It can be anything. We could have replaced *spice* with *energy... catalyst... platinum...* and no one will be any the wiser. Earl Ward Plummer [2] wrote along the same line, "*... whoever controls complex materials controls science and technology,* i.e., progress is *materials-driven...*" Complex materials exhibit startling properties, reveal new and unexpected insights. Development of methods and models to synthesize and simulate complex systems would prove to be extremely useful. But, don't fall into the trap of developing sophisticated experimental and theoretical techniques becoming an end in itself: one better measurement, one better calculation. Remember Ockham's Razor? Philip Warren Anderson [3] wrote, " *... a simplified model throws more light on the real workings of nature than any number of 'ab initio' calculations ..., which, even where correct, often contain so much detail as to conceal rather than reveal reality… After all, the perfect computation simply reproduces nature, it does not explain her ...*" "*Resources are the enemy of imagination,*" quipped Thomas Delavane in the 2012 TV series adaptation of James Patterson's 2012 novel ***Zoo*** [4]. With these in mind, at the workshop, we will cite some hydrogen-surface reaction related case studies, and introduce some insights gained from *spice*-related studies (cf., e.g., [5-7]), in our quest to Realize Designer Materials utilizing Surface as a Foundation, and explore some physical phenomena along the way.

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Theoretical Study of Hydrogenation Process of CO_2 on Metal Catalysts

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Abstract

Chemical reactions at surfaces and interfaces play important roles in wide ranges of applications such as hegerogeneous catalysis, electrochemistry, fuel cells, batteries, etching processes of semiconductor materials, and so on. In this talk, we will present theoretical investigation and prediction of hydrogenation of CO2 over Cu catalyst[1,2]. Adsorption and reaction of CO2 on solid surfaces are attracting growing interest because of their importance in industrial, energy and environmental management. To clarify reaction mechanisms and to identify important factors governing the reactivity of CO2 on solid surfaces are very important to develop more efficient catalysts or catalytic processes for utilization of CO2. To this end, we investigated CO2 adsorption and hydrogenation[1] on Cu surfaces using van der Waals density functionals as implemented in our home made STATE (Simulation tool for Atom TEchnology) program code [3]. We theoretically proposed a new reaction scheme to enhance the hydrogenation of CO2 on Cu.

In the second topic, we will discuss the catalytic dry reforming of methane (DRM) [4]. The emissions of greenhouse gases (CH4 and CO2) are rising exponentially due to human activities and increased energy demand, contributing to global warming and climate changes. To make use of CH4 and CO2 into renewable energy, catalytic DRM is an efficient pathway to convert them into syngas (CO and H2). Currently, supported Ni could be the most studied catalyst due to its relatively high activity and low cost. However, the efficiency of Ni is widely known to be easily suppressed by carbon deposition. In this study, we investigate the surface reactions of CO2 with C* at the flat and step sites of face-centered cubic (FCC) Co ((111), (110), (100), (211), and (221)), which represent the major surfaces of Co nanoparticles.

References

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HLA Polymorphism in SCAR Reaction to Allopurinol Drug for Gout Treatment

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Abstract

ALP, a xanthine oxidase inhibitor, is an FDA-approved urate-lowering medication used to treat Gout, to prevent tumor lysis syndrome, and to prevent recurrent calcium nephrolithiasis in hyperuricosuria patients. However, it has been known as a common cause of severe cutaneous adverse drug reactions (SCAR) including Stevens-Johnson syndrome, toxic epidermal necrolysis, hypersensitivity syndrome/drug reaction with eosinophilia and systemic symptoms, especially in patients carrying the Human Leukocyte Antigens allele HLA-B*58:01, which is more prevalent in Asian population [1]. However, although patients who do not carry the HLA-B*58:01 allele, they still exhibit allopurinol-induced SCAR. Specifically, a clinical trial at Bach Mai Hospital, Viet Nam shows that many of these patients have the HLA-A*24:02, HLA-A*33:03, HLA-A*02:03, HLA-A*11:01, HLA-A*29:01, HLA-A*26:01…alleles [2-3], not only have a high odd ratio but also have the most common frequencies in Vietnam. In this work, using computational molecular dynamics simulation method, we investigated the binding of ALP at two active sites of the HLA protein, consisting of the binding pockets F and B to alleles. The results are compared with the binding affinity of ALP to the control allele HLA-B*58:01, the standard allele for ALP allergy. Our results showed that only five complexes of five alleles and ALP at the binding pocket F were stable after 100ns simulation time. ALP had strong interactions with three important residues located in the binding pocket F of each allele, which include the seven amino acid residues 76, 77, 81, 95, 96, 116, and 123 - these are also the key residues in the binding pocket F. The hydrogen interaction plays a role in holding the ligand and stabilizing the spatial structure of the complex in five HLA systems. All six systems' binding free energy between ligand and protein fell below the threshold of – 9 to – 15 kcal/mol, suggesting that ALP has a strong binding affinity for all five alleles. This data suggests that ALP has a strong binding affinity for two alleles HLA-A*24:02 and HLA-A*33:03. Thus, in addition to HLA-B*58:01, the alleles HLA-A*24:02, HLA-A*33:03 may be a potential screening marker before prescribing Allopurinol for Gout treatment, to reduce the risk of not only SCARs but also MCARs.

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First-Principles Study of Electronic and Optical Properties of Au/LaAlO3/SrTiO3 Heterointerface

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Abstract

The heterointerface of Au/$LaAlO_3$/$SrTiO_3$ is promising for spintronics and optoelectronics applications. However, no works are available to elucidate the electronic and optical properties of this heterointerface. Therefore, we clarified the mentioned properties using density functional theory calculations. We will share our new findings in the workshop.

In Silico Studies of Monolayer Systems

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Abstract

Density functional theory (DFT) calculations performanced in high-performance computing cluster (HPCC) are used to investigate essential properties of carbon-doped silicene nanoribbons (SiNR). Through the DFT calculations, a complete first-principles theoretical framework is developed to fully characterize the carbon-enriched properties include the formation energies, optimal lattice parameters, phonon spectrum, orbital- and atom-decomposed electronic band structures, orbital- and atom-projected density of states (DOSs), spatial charge density distributions, and charge density difference along with various directions. Under C substitution effects, atomic configurations of the single C substitutions, double C substitutions under different adatom distributions of ortho, meta, and para, and full C substitutions are included in calculations, in which buckling of the pristine system is much reduced under the single and double C configurations that becomes a flat structure under the full C configuration. The calculated formation energies and phonon spectrum evidence that all carbon substiution configurations achieve good structural stability. The typical hybridization mechanism of the quasi σ of Si-($3s,3p_x,3p_y$) and C-($2s,2p_x,2p_y$) and the quasi π of Si-$3p_z$ and C-$2p_z$ is formed in very strong Si-C bonds that lead to stable structures. As a close relationship, the C-diversified structures result in diverse electronic properties, in which the bandgap of the pristine system is almost opened under various C configurations. The largest opened bandgap of 2.37 eV is found at the full C configuration that is determined by quasi π bands of the highest occupied valence band of C-$2p_z$ and lowest unoccupied conduction band of Si-$3p_z$. The C-enriched properties of SiNR can be very potential for applications in optoelectronic devices. Besides, the C substitution-induced typical hybridization mechanism of the quasi σ and π orbitals that has been realized by the completely developed theoretical framework in this study can be fully generalized to other monolayer systems.

Keywords: Formation energies, phonon spectrum, electronic band structures, high-performance calculations, DFT studies, carbon substitutions, complex orbital hydridization, and charge density distributions.

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