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

Thu Dau Mot University, Binh Duong Province, Vietnam

April 14th-16th, 2022

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

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

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

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

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

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

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

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

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

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

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**		
08:00-08:25, **VIP 1** **Opening remarks** Prof. Nguyen Van Hiep, Thu Dau Mot University Prof. Yoshitada Morikawa, Osaka University 08:25-08:30: **VIP 1** **Group Picture** 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** Prof. Sato Kazunori, Osaka University 10:40-11:40, **HPC.R** **Hands-on Tutorial 1 (AkaiKKR)** Prof. Sato Kazunori, Osaka University	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)** Prof. Ikutaro Hamada and Prof. Yoshitada Morikawa, Osaka University
Lunch (1h20 mins)	**Lunch (1h20 mins)**	**Lunch (1h20 mins)**
13:00-15:00, **HPC.R** **Hands-on Tutorial 1 (AkaiKKR)** 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) Prof. Ikutaro Hamada and Prof. Yoshitada Morikawa, Osaka University

		Break (10 mins)
Chair: 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 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 Prof. Nguyen Thanh Tien, Can Tho University	Chair: 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 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 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 Prof. Vo Van On, Thu Dau Mot University