

## CURRICULUM VITAE

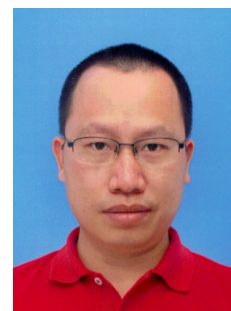
### NGUYEN TIEN QUANG

#### Affiliation:

Osaka University  
Institute for NanoScience Design  
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#### Research Keywords:

•Computational Physics/Chemistry •Computational Materials Science •Condensed Matter Physics  
•Molecular Electronic Devices •Reactions on Surfaces •Diffusion in Metals and Alloys •Iron-Carbon Alloys  
•High-Entropy Alloys •Lattice Thermal Conductivity  
•Multi-Scale Modelling •First-Principles Calculation •Molecular Dynamics •Monte Carlo/Kinetic Monte Carlo  
•Cluster Expansion/Variation Method •Evolutionary Algorithm •Interatomic Potential Development

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## PERSONAL DETAILS

- **Full Name:** TIEN QUANG, NGUYEN
  - **Gender:** Male
  - **Date of Birth:** October 06, 1982
  - **Language Proficiency:** Vietnamese (native), English (fluent), Japanese (basic)
- Nationality:** Vietnam  
**Marital Status:** Married  
**Place of Birth:** Binh Phuoc, Vietnam

## EDUCATIONAL HISTORY

- **10/2010 - 09/2013: Osaka University (Graduate School of Engineering)**  
Quantum Engineering Design Program  
**Degree and Major:** Doctor of Philosophy in Engineering  
**Dissertation:** “*Theoretical Study on Nitric Oxide Adsorption and Oxidation on Metallo-Macrocycles and Ceria-Supported Platinum Cluster*”  
**Supervisor:** Prof. Hideaki Kasai
- **10/2008 - 09/2010: Osaka University (Graduate School of Engineering)**  
Quantum Engineering Design Program  
**Degree and Major:** Master of Engineering  
**Dissertation:** “*Adsorption of Nitric Oxide on Metal Porphyrin Tape: The Role of Metal Porphyrin Tape as Sensor in Detecting Nitric Oxide Gas*”  
**Supervisor:** Prof. Hideaki Kasai
- **01/2007 - 12/2007: Osaka University (Graduate School of Engineering)**  
JASSO Exchange Student Program  
**Supervisor:** Prof. Hideaki Kasai
- **12/2004 - 12/2006: Vietnam National University in Hanoi (VNU University of Science)**  
**Degree and Major:** Master of Science in Theoretical Physics  
**Dissertation:** “*DFT Study on The Electronic Properties of Perovskite*”  
**Supervisor:** Prof. Bach Thanh Cong
- **09/2000 - 06/2004: Vietnam National University in Hanoi (VNU University of Education)**  
Teacher Licensure Program  
**Degree and Major:** Bachelor of Science in Physics/Physics Education  
**Dissertation:** “*Quantum Visualization of Hydrogen Atom*”  
**Supervisor:** Prof. Le Viet Du Khuong

## EMPLOYMENT HISTORY

- **12/2015 - present: Osaka University (Institute for NanoScience Design)**  
(Professional development Consortium for Computational Materials Scientists)

**Position:** Specially-Appointed Assistant Professor (full-time)

**Duties:** Doing research on Atomistic Materials Design of New Heterogeneous Iron/Steel

- **12/2013 - 12/2015: Osaka University (Graduate School of Engineering Science)**  
**Position:** Postdoctoral Researcher (full-time)  
**Duties:** Doing research on Hydrogen Behavior in Iron/Steel
- **10/2013 - 11/2013: Osaka University (Graduate School of Engineering)**  
**Position:** Postdoctoral Researcher (part-time)  
**Duties:** Doing research on Diesel Oxidation Catalysts
- **01/2008 - 09/2008: Osaka University (Graduate School of Engineering)**  
**Position:** Specially-Appointed Researcher (full-time)  
**Duties:** Doing research on Molecular Electronic Devices and Diesel Oxidation Catalysts
- **06/2004 - 12/2006: Vietnam National University in Hanoi (VNU University of Science)**  
**Position:** Teaching Assistant (part-time)  
**Duties:** Instruction for undergraduate students on MATLAB practice tutorials

## TEACHING EXPERIENCE

- **10/2017 - present: Vietnam-Japan University (Master's Program in Nanotechnology)**  
**Duties:** Teaching master course students and supervising students' theses
- **05/2017 - 06/2017: Vietnam-Japan University (Master's Program in Nanotechnology)**  
**Duties:** Teaching master course students

## RESEARCH EXPERIENCE

- **Materials Design of New Thermoelectric Materials:**  
Investigation into the unusual behaviors in electron and lattice thermal conductivity of Fe-doped  $\text{Si}_x\text{Ge}_{1-x}$  to improve their thermoelectric efficiency by using first-principles calculations and non-equilibrium/equilibrium molecular dynamics (NEMD/EMD); Development of new Tersoff potential for molecular dynamics simulations of Si-Ge-Fe system.
- **Atomistic Materials Design of New Heterogeneous Iron/Steel:**  
Study of the ferrite/martensite phase transformation, the diffusion properties as well as the clustering of carbon in steel by using kinetic Monte Carlo, first-principles calculations, molecular dynamics and cluster expansion/variation methods; Development of new Tersoff/ZBL potential for molecular dynamics and kinetic Monte Carlo simulations of Fe-C system.
- **Hydrogen Behavior in Iron/Steel:**  
Study of the hydrogen interaction with various defects (vacancies, grain boundaries,...) and solutes (carbon,...) in steel by using first-principles and molecular dynamics methods; Development of new Embedded-Atom Method (EAM) potential for molecular dynamics simulations of Fe-C-H system.
- **Diesel Oxidation Catalysts:**  
Study of the oxidation/reduction processes of harmful gases on metal surfaces and metal oxide supported metal clusters for heterogeneous catalysis applications by using DFT+U and ab-initio molecular dynamics methods.
- **Molecular Devices:**  
Study of the electronic and magnetic properties of various metallo-macrocycles (porphyrin, phthalocyanine,...) and their interactions with diatomic gases for sensor applications by using first-principle methods.
- **Fuel Cells:**  
Study of the oxidation processes on bimetallic surfaces for renewable energy applications by using first-principles and Monte Carlo methods.

## INDUSTRIAL COLLABORATION

- **ISMA Project:** Hydrogen Behavior in Iron/Steel (2013-2015)

- **TANAKA** Precious Metals Group Project: Cathode Catalysts for Fuel Cells (2013)
- **ISUZU** Motor Inc. Project: Diesel Oxidation Catalyst for Car Exhaust Filters (2008-2013)
- **SHARP** Corporation Project: Molecular Electronic Devices for Gas Sensors (2007-2009)

## HONORS/AWARDS

- **2013:** Premium Doctor Degree (conferred by Osaka University - Global Center of Excellence (GCOE) “Atomically Controlled Fabrication Technology” Program) for obtaining extra credits on the experimental techniques in solid state physics and surface science.
- **2012:** Best Poster Award for the presentation entitled “*Spin effects in metal surface reaction: O<sub>2</sub> on ferromagnetic Pt/M*” at the 54<sup>th</sup> Annual Symposium of the Vacuum Society of Japan
- **2011:** Best Poster Award for the presentation entitled “*Study of NO oxidation reaction over Pt cluster supported on  $\gamma$ -Al<sub>2</sub>O<sub>3</sub>(111) surface*” at the 4<sup>th</sup> International Symposium on Atomically Controlled Fabrication Technology
- **2009:** IOP Select Paper: JPCM Top Papers for the article entitled “*Another way of looking at bonding on bimetallic surfaces: The role of spin polarization of surface metal d-states*”
- **2008:** 5-year MEXT Scholarship (offered by Japanese Ministry of Education, Culture, Sports, Science and Technology under Quantum Engineering Design Program)
- **2007:** 1-year JASSO Scholarship (offered by Japan Student Services Organization under Student Exchange Support Program)
- **2003:** VNU Outstanding Young Face Award (conferred by Vietnam National University, Hanoi) for the remarkable achievements in study and social activities
- **2001:** VNU Outstanding Young Face Award (conferred by Vietnam National University, Hanoi) for the remarkable achievements in study and social activities

## GRANTS/FELLOWSHIPS

- Japanese Ministry of Education, Culture, Sports, Science and Technology (MEXT) Scholarship under Quantum Engineering Design Program (10/2008-09/2013)
- Japan Student Services Organization (JASSO) Scholarship under Student Exchange Support Program (01-12/2007)
- Japan GCOE (Global Center of Excellence) Program - Small Group Projects:
  - Tien Quang Nguyen, Ferensa Oemry, Saputro Adhitya Gandaryus, Koji Shimizu and Chong Kong Ng. “*A theoretical study of dynamics and characteristics of oxygen reduction reaction for new catalyst development*” (2012-2013)
  - Tien Quang Nguyen, Aspera Susan Meñez, Wungu Triati Dewi Kencana, Moreno Joaquin Lorenzo Valmorla, Saputro Adhitya Gandaryus and Yohei Ushijima. “*The theoretical analysis on the application to electronic devices using organic materials*” (2011-2012)
  - Tien Quang Nguyen, Hirofumi Kishi, Mary Clare Sison Escaño, Abdulla Ali Abdulla Sarhan and Ferensa Oemry. “*Design of thin film nano-devices using simulation technology*” (2009-2010)

## RESEARCH FUNDS

### Fiscal Year 2019:

**Building of Consortia for the Development of Human Resources in Science and Technology**  
Supported by MEXT (Japan)  
**Research Grant:** 1,000,000JPY

### Fiscal Year 2018:

**Building of Consortia for the Development of Human Resources in Science and Technology**  
Supported by MEXT (Japan)  
**Research Grant:** 4,000,000JPY

### Fiscal Year 2017:

**Building of Consortia for the Development of Human Resources in Science and Technology**  
Supported by MEXT (Japan)  
**Research Grant:** 2,000,000JPY

### Fiscal Year 2016:

**Building of Consortia for the Development of Human Resources in Science and Technology**  
Supported by MEXT (Japan)  
**Research Grant:** 1,000,000JPY

**Fiscal Year 2015:****Building of Consortia for the Development of Human Resources in Science and Technology**

Supported by MEXT (Japan)

**Start-up Funding Grant:** 6,620,000JPY**PUBLICATIONS****Patent(s):****Title (short):** “Method of manufacturing chemical substance sensing element”**Title (full):** “Manufacturing method of chemical substance sensing element, involves including process of selecting material predicted to be suitable for surface modification material of electro-conductive substrate from candidate material”**Language:** Japanese**Patent Number:** JP2011080798-A**Published Date:** 21 April, 2011**Inventor(s):** T. Q. NGUYEN, M. OTONASHI, T. KAWATA, M. YAMANAKA, K. HARA, H. KASAI, H. NAKANISHI**International Patent Classification:** G01N-027/12 (or G01N 27/12)**Review Articles and Books:**

1. Mary Clare Sison Escano, Tien Quang Nguyen and Hideaki Kasai  
“Fundamentals of electronic modification of graphene by Si and H”  
Chapter 23, Graphene Science Handbook: Size-Dependent Properties  
Taylor & Francis Group, USA (2016) 351-368 (ISBN: 9781466591356)
2. Tien Quang Nguyen, Mary Clare Sison Escano and Hideaki Kasai  
“Porphyrins: Chemistry, properties and applications”  
Chapter 6, Handbook of Porphyrins: Chemistry, Properties and Applications  
Nova Science Publishers, USA (2012) 229-260 (ISBN: 978-1-62081-068-2)

**Original Articles (Peer-Reviewed, Under Review...):**

1. Ryo Yamada, Akira Masago, Tetsuya Fukushima, Hikari Shinya, Tien Quang Nguyen and Kazunori Sato  
“First-principles calculation of electronic density of states and Seebeck coefficient in transition-metal-doped Si-Ge alloys”  
Applied Physics Express (*Under Review*) - <https://arxiv.org/abs/2001.10191>
2. Mary Clare Sison Escano and Tien Quang Nguyen  
“Does GaAs bulk lattice really expand due to defects in the low concentration regime?”  
Solid State Communications (*Under Review*)
3. Mary Clare Sison Escano, Maria Herminia Balgos, Tien Quang Nguyen, Elizabeth Ann Prieto, Elmer Estacio, Arnel Salvador, Armando Somintac, Rafael Jaculbia, Norihiko Hayazawa, Yousoo Kim and Masahiko Tani  
“True bulk As-antisite defect in GaAs(110) identified by DFT calculations and probed by STM/STS measurements”  
Applied Surface Science (*In Press*) - <https://doi.org/10.1016/j.apsusc.2020.145590>
4. Tien Quang Nguyen, Mary Clare Sison Escano, Kazunori Sato, Yoji Shibutani, Tamio Oguchi and Tetsuo Mohri  
“Atomic and effective pair interactions in FeC alloy with point defects: A cluster expansion study”  
ISIJ International **59** (2019) 2343-2351
5. Mary Clare Sison Escano, Tien Quang Nguyen, Yu Osanai, Hideaki Kasai and Masahiko Tani  
“Large-scale spin-polarized DFT calculation of electronic properties of GaAs with defects”  
Materials Research Express **6** (2019) 055914(1-8)
6. Tien Quang Nguyen, Kazunori Sato and Yoji Shibutani  
“Development of Fe-C interatomic potential for carbon impurities in  $\alpha$ -iron”  
Computational Materials Science **150** (2018) 510-516
7. Tien Quang Nguyen, Kazunori Sato and Yoji Shibutani  
“First-principles study of BCC/FCC phase transition promoted by interstitial carbon in iron”  
Materials Transactions **59** (2018) 870-875
8. Mary Clare Sison Escano, Tien Quang Nguyen and Hideaki Kasai  
“Spin-up “pristine-like” Dirac cone in bridge-structure graphene on Ni(111)”  
Applied Surface Science, **427** (2018) 949-952
9. Mary Clare Sison Escano, Tien Quang Nguyen and Hideaki Kasai  
“Another way of looking at reactivity enhancement in large-area graphene: The role of exchange splitting from first-principles methods”  
Journal of Physical Chemistry C, **119** (2015) 26636-26642

10. Nguyen Hoang Linh, Tien Quang Nguyen, Wilson Agerico Dino and Hideaki Kasai  
*"Effect of oxygen vacancy on the adsorption of O<sub>2</sub> on anatase TiO<sub>2</sub>(001): A DFT-based study"*  
 Surface Science, **633** (2015) 38-45
11. Tien Quang Nguyen, Mary Clare Sison Escano, Hiroshi Nakanishi, Hideaki Kasai, Hiroyoshi Maekawa, Kazuo Osumi and Kaoru Sato  
*"DFT+U study on the oxygen adsorption and dissociation on CeO<sub>2</sub>-supported platinum cluster"*  
 Applied Surface Science, **288** (2014) 244-250
12. Tien Quang Nguyen, Allan Abraham Bustria Padama, Mary Clare Sison Escano and Hideaki Kasai  
*"Theoretical study on The adsorption of NO on metal macrocycles, Metal = Mn, Fe, Co, Ni, Cu, Zn"*  
 ECS Transactions, **45** (2013) 91-100
13. Mary Clare Sison Escano, Tien Quang Nguyen and Hideaki Kasai  
*"Molecular oxygen adsorption on ferromagnetic platinum"*  
 Chemical Physics Letters, **555** (2013) 125-130
14. Hirofumi Kishi, Ferensa Oemry, Tien Quang Nguyen, Shinichi Kunikata, Hiroshi Nakanishi, Hideaki Kasai, Hiroyoshi Maekawa and Kazuo Osumi  
*"Study of NO oxidation reaction over the Pt cluster supported on  $\gamma$ -Al<sub>2</sub>O<sub>3</sub>(111) surface"*  
 Current Applied Physics, **12** (2012) S110-S114
15. Mary Clare Sison Escano, Tien Quang Nguyen and Hideaki Kasai  
*"Analysis of band gap formation in graphene by Si impurities: Local bonding interaction rules"*  
 Chemical Physics Letters, **515** (2011) 85-90
16. Mary Clare Sison Escano, Tien Quang Nguyen and Hideaki Kasai  
*"Molecular and electronic tuning of Si/CNT hybrid system"*  
 Japanese Journal of Applied Physics, **50** (2011) 045101(1-4)
17. Tien Quang Nguyen, Mary Clare Sison Escano and Hideaki Kasai  
*"Nitric oxide adsorption effects on metal phthalocyanines"*  
 Journal of Physical Chemistry B, **114** (2010) 10017-10021
18. Mary Clare Sison Escano, Tien Quang Nguyen, Hiroshi Nakanishi and Hideaki Kasai  
*"Another way of looking at bonding on bimetallic surfaces: The role of spin polarization of surface metal d-states"*  
 Journal of Physics: Condensed Matter, **21** (2009) 492201(1-6)
19. Tien Quang Nguyen, Susan Menez Aspera, Hiroshi Nakanishi and Hideaki Kasai  
*"NO adsorption effects on various functional molecular nanowires"*  
 Computational Materials Science, **47** (2009) 111-120
20. Tien Quang Nguyen, Mary Clare Sison Escano, Reiko Tanaka, Hiroshi Nakanishi and Hideaki Kasai  
*"The adsorption of NO on various metal tape-porphyrins: A first-principles study"*  
 Journal of the Physical Society of Japan, **78** (2009) 014706(1-9)
21. Mary Clare Sison Escano, Tien Quang Nguyen, Hiroshi Nakanishi and Hideaki Kasai  
*"Bonding of Pt/Fe overlayer and its effects on atomic oxygen chemisorption from density functional theory study"*  
 Surface Science, **602** (2008) 3415-3423
22. Tien Quang Nguyen, Mary Clare Sison Escano, Nobuaki Shimoji, Hiroshi Nakanishi and Hideaki Kasai  
*"Adsorption of diatomic molecules on iron tape-porphyrin: A comparative study"*  
 Physical Review B, **77** (2008) 195307(1-7)
23. Tien Quang Nguyen, Mary Clare Sison Escano, Nobuaki Shimoji, Hiroshi Nakanishi and Hideaki Kasai  
*"DFT study on the adsorption of NO on iron tape-porphyrin"*  
 Surface and Interface Analysis, **40** (2008) 1082-1084
24. Tien Quang Nguyen and Thanh Cong Bach  
*"First-principles calculation for BaTiO<sub>3</sub>"*  
 Communications in Physics, **17** (2007) 128-133

#### **Other Articles (Proceedings, Bulletin...):**

1. Tien Quang Nguyen, Ngoc Nam Ho, Kazunori Sato, Yoji Shibutani  
*"Atomistically kinetic simulations of carbon diffusion in  $\alpha$ -Fe with point defect"*  
 Proceedings of the Computational Mechanics Conference, Volume **32** (2019) 250 (Online ISSN: 2424-2799)
2. Ngoc Nam Ho, Tien Quang Nguyen and Yoji Shibutani  
*"Atomistically kinematic properties of carbon diffusion in alpha iron with point defects"*  
 Proceedings of the Vietnam-Japan Science and Technology Symposium 2019 (06/05/2019, Vietnam-Japan University)
3. Tien Quang Nguyen, Ngoc Nam Ho, Thi Thu Dinh Ngo, Kazunori Sato and Yoji Shibutani  
*"Diffusion properties of carbon in Fe-C alloy using new Tersoff potential"*  
 Proceedings of the Computational Mechanics Conference, Volume **31** (2018) 237 (Online ISSN: 2424-2799)

- Mary Clare Sison Escano, Tien Quang Nguyen, Hiroshi Nakanishi and Hideaki Kasai  
*"Controlling oxidation reaction on platinum by spin manipulation"*  
 Technical Proceedings of the 2012 NSTI Nanotechnology Conference and Expo, Volume 2 (2012)  
 645-648 (ISBN: 978-1-4665-6275-2)

#### Teaching Resource(s):

**Course Name:** *"Introduction on Molecular Dynamics simulation"*

**Objectives:** This course helps the students to understand about the basic of molecular dynamics method and simulation, and to know how to use LAMMPS as a computational tool to do their research.

**Constructed Materials:** Lecture notes, lecture slides, hands-on examples and exams.

**Teaching Level:** Graduate students

## PRESENTATIONS

#### Invited Lectures and Seminars:

- "Kinetic Monte Carlo simulations of carbon diffusion in bcc iron with point defects"*  
 Scientific Seminar at Institute for Materials Research  
 (08/10/2019, Tohoku University, Miyagi, Japan)
- "Atomistically kinetic simulations of carbon behavior in bcc iron with point defect"*  
 Short-talk Session at the 35<sup>th</sup> Computational Materials Design  
 (02-06/09/2019, Osaka University, Osaka, Japan)
- "Diffusion properties of carbon and tetragonality effect in Fe-C alloy"*  
 Scientific Seminar at Institute for Materials Research  
 (06/12/2018, Tohoku University, Miyagi, Japan)
- "Computational kinetics on diffusion of carbons in bcc iron"*  
 Scientific Seminar at Institute for Materials Research  
 (07/06/2018, Tohoku University, Miyagi, Japan)
- "Analytic interatomic potential for modeling phase transformation in the Fe-C system"*  
 Scientific Seminar at Institute for Materials Research  
 (02/08/2017, Tohoku University, Miyagi, Japan)
- "Analytic bond-order potential for atomistic simulations of Fe-C system"*  
 Scientific Seminar at Center for Computational Materials Science, Institute for Materials Research  
 (18/01/2017, Tohoku University, Miyagi, Japan)
- "Interatomic potentials development of Fe-C binary system for atomistic materials design of new heterogenous iron"*  
 Scientific Seminar at Faculty of Physics  
 (04/11/2016, Hanoi National University of Education, Hanoi, Vietnam)
- "Development of interatomic potentials for modeling of hydrogen and carbon interaction near lattice defects in bcc iron"*  
 Scientific Seminar at Center for Atomic and Molecular Technologies, Graduate School of Engineering  
 (28/04/2016, Osaka University, Osaka, Japan)
- "First-principles study on NO adsorption and oxidation on metallo-macrocycles and ceria-supported Pt cluster"*  
 Mini Symposium on Computational Chemistry for Material Applications  
 (15-16/07/2013, The National University of Malaysia, Selangor, Malaysia)
- "Computational Materials Design for energy and environmental applications"*  
 Scientific Seminar at Faculty of Physics  
 (06-08/12/2012, VNU University of Science, Hanoi, Vietnam)
- "Porphyrins and macrocycles: From basics to applications"*  
 ECS 221<sup>st</sup> Meeting  
 (06-10/05/2012, Washington State Convention Center, Seattle, Washington, USA)

#### Lectures for Graduate Students:

- "Nanomechanics: Introduction on Molecular Dynamics simulation"*  
 Lecture and hands-on practice for master course students in Nanotechnology Program, VJU  
 (01-08/12/2019, Vietnam Japan University, Hanoi, Vietnam)
- "Nanomechanics: Introduction on Molecular Dynamics simulation"*  
 Lecture and hands-on practice for master course students in Nanotechnology Program, VJU  
 (20-27/12/2018, Vietnam Japan University, Hanoi, Vietnam)
- "Nanomechanics: Introduction on Molecular Dynamics simulation"*  
 Lecture and hands-on practice for master course students in Nanotechnology Program, VJU  
 (25/11-11/12/2017, Vietnam Japan University, Hanoi, Vietnam)
- "Nanomechanics: Introduction on Molecular Dynamics simulation"*



Lecture and hands-on practice for master course students in Nanotechnology Program, VJU  
(08-22/05/2017, Vietnam Japan University, Hanoi, Vietnam)

**Oral Presentations in International Conferences:**

1. “Carbon diffusion and clustering in bcc iron: A kinetic Monte Carlo study”  
Workshop on Nanotechnology-Driven Topics  
(10/12/2019, Osaka University, Osaka, Japan)
2. “Atomistic simulations of carbon behavior in bcc iron with point defect”  
PCoMS Symposium & Annual Meeting of Supercomputing Consortium for Computational Materials Science 2019  
(24-25/10/2019, Tohoku University, Miyagi, Japan)
3. “Atomistically kinetic simulations of carbon diffusion in  $\alpha$ -Fe with point defect”  
The 32<sup>nd</sup> Meeting on Computational Mechanics of the Japan Society of Mechanical Engineers  
(16-18/09/2019, Toyo University, Saitama, Japan)
4. “Cluster Expansion simulations of Fe-C alloys with point defects: Atomic and effective cluster interactions”  
The 164<sup>th</sup> Annual Spring Meeting of The Japan Institute of Metals and Materials  
(20-22/03/2019, Tokyo Denki University, Tokyo, Japan)
5. “Diffusion properties of carbon in Fe-C alloy using new Tersoff potential”  
The 31<sup>st</sup> Meeting on Computational Mechanics of The Japan Society of Mechanical Engineers  
(23-25/11/2018, Tokushima University, Tokushima, Japan)
6. “Diffusion properties of carbon in  $\alpha$ -Fe”  
PCoMS Symposium & Annual Meeting of Supercomputing Consortium for Computational Materials Science 2018  
(22-23/10/2018, Tohoku University, Miyagi, Japan)
7. “Cluster Expansion Method study on the effective interaction in Fe-C alloys”  
The 163<sup>rd</sup> Annual Fall Meeting of The Japan Institute of Metals and Materials  
(19-21/09/2018, Tohoku University, Miyagi, Japan)
8. “Construction of interatomic potential for Fe-C systems using evolutionary algorithm”  
APS March Meeting 2018  
(04-09/03/2018, Los Angeles Convention Center, Los Angeles, California, USA)
9. “Interatomic potentials for carbon in iron based on density functional theory”  
PCoMS Symposium & Annual Meeting of Supercomputing Consortium for Computational Materials Science 2017  
(09-10/11/2017, Tohoku University, Miyagi, Japan)
10. “New atomic potential of Fe-C binary system for phase transformation of heterogeneous materials”  
The 161<sup>th</sup> Annual Fall Meeting of The Japan Institute of Metals and Materials  
(06-08/09/2017, Hokkaido University, Hokkaido, Japan)
11. “Atomistic materials design of new iron with highly-tuned strength, ductility and fracture toughness: Interatomic potentials development for Fe-C binary system”  
PCoMS Symposium & Annual Meeting of Supercomputing Consortium for Computational Materials Science 2016  
(17-18/10/2016, Tohoku University, Miyagi, Japan)
12. “Interatomic potentials for modeling hydrogen and carbon interaction near lattice defects in the Fe-C-H system”  
International Workshop on Quantum Engineering Design: Materials Design and Realization  
(24-26/03/2016, Osaka University, Osaka, Japan)
13. “Atomistic materials design of new iron with highly-tuned strength, ductility and fracture toughness: Interatomic potential development”  
PCoMS Kick-off Meeting  
(26/02/2016, Tohoku University, Tokyo, Japan)
14. “NO oxidation on CeO<sub>2</sub>-supported Pt<sub>4</sub> cluster: A DFT+U study”  
Quantum Engineering Design Workshop  
(25/10/2013, Osaka University, Osaka, Japan)
15. “NO oxidation on O pre-covered Pt<sub>4</sub>/CeO<sub>2</sub>”  
OU-TUM Workshop: Trends in Catalysis  
(16/05/2013, Osaka University, Osaka, Japan)
16. “Theoretical Investigation on NO oxidation on O pre-covered Pt<sub>4</sub>/CeO<sub>2</sub>”  
International Workshop on The Theory of Dense Kondo Systems  
(19-20/03/2013, Osaka University, Osaka, Japan)
17. “DFT+U investigation on the adsorption and dissociation of oxygen on Pt-coated Ceria”  
International Workshop on Current Surface Science Trend  
(08/11/2012, Osaka University, Osaka, Japan)

18. “*Oxidation of metal and metal oxide systems*”  
Asia Computational Materials Design Workshop  
(10-12/10/2011, De La Salle University, Manila, Philippines)
19. “*Computational Materials Design case studies: Oxidation of metal/metal oxide systems*”  
International Conference on Quantum Simulations and Design  
(27-29/09/2011, Max Planck Institute, Dresden, Germany)
20. “*First-principles study on nitric oxide adsorption on metal tape-porphyrines*”  
Asia Computational Materials Design Workshop  
(15-17/02/2011, Mahidol University, Bangkok, Thailand)
21. “*Adsorption of nitric oxide on metal porphyrin tape*”  
Asia Computational Materials Design Workshop  
(16-18/12/2010, Hue University, Hue, Vietnam)
22. “*Computational Materials Design of molecular bridge systems for potential applications as nano-electronics devices*”  
International Conference on Core Research and Engineering Science of Advanced Materials & Third International Conference on Nanospintronics Design and Realization  
(30/05-04/06/2010, Osaka University, Osaka, Japan)
23. “*Nitric oxide adsorption effects on metal phthalocyanines*”  
OU-DLSU Academic Research Workshop  
(27-28/05/2010, Osaka University, Osaka, Japan)
24. “*The role of metal porphyrin tape as sensor in detecting NO gas*”  
Asia Computational Materials Design Workshop  
(26-28/11/2009, Ha-Noi University of Science, Ha-Noi, Vietnam)
25. “*NO adsorption effects on metal tape-porphyrins*”  
GCOE International Workshop  
(25-27/11/2008, Osaka University, Osaka, Japan)
26. “*The adsorption of NO on various metal tape-porphyrins*”  
ITB-OU Academic Research Workshop  
(30/06/2008, Osaka University, Osaka, Japan)
27. “*DFT study on the binding of CO, NO, and O<sub>2</sub> to iron tape-porphyrin*”  
International Workshop on Quantum Simulation 2007  
(13/09/2007, Osaka University, Osaka, Japan)
28. “*O<sub>2</sub> adsorption effects on electronic properties of Fe tape-porphyrin*”  
International Science and Engineering Workshop  
(15/05/2007, Osaka University, Osaka, Japan)
29. “*DFT study on O<sub>2</sub> adsorbed Fe tape-porphyrin*”  
The 3<sup>rd</sup> International Workshop on Reactions Involving Oxygen  
(10/05/2007, Osaka University, Osaka, Japan)
30. “*Study of electronic properties of perovskite BaTiO<sub>3</sub>*”  
The 4<sup>th</sup> Workshop on Simulation & Modeling Physics  
(22-24/11/2006, Institute of Physics, Ha-Noi, Vietnam)

#### **Poster Presentations in International Conferences:**

1. “*Diffusion of carbon in  $\alpha$ -Fe in the presence of vacancy*”  
The 22<sup>th</sup> Asian Workshop on First-Principles Electronic Structure Calculations (ASIAN-22)  
(28-30/10/2019, Osaka University, Osaka, Japan)
2. “*Hydrogen and carbon interactions near lattice defects in bcc iron by combined theoretical methods*”  
2015 MRS Fall Meeting & Exhibit  
(29/11-04/12/2015, Boston, Massachusetts, USA)
3. “*Atomistic modeling of hydrogen-vacancy-carbon interaction in  $\alpha$ -iron*”  
The 9<sup>th</sup> International Conference on Computational Physics  
(07-11/01/2015, The National University of Singapore, Singapore)
4. “*Hydrogen-vacancy-carbon formation in bcc iron: First-principles study*”  
The 9<sup>th</sup> General Meeting of Asian Consortium on Computational Materials Science - Virtual Organization  
(20-22/12/2014, Okinawa Institute of Science and Technology, Okinawa, Japan)
5. “*NO oxidation on oxygen pre-covered Pt<sub>n</sub>/CeO<sub>2</sub>(111)*”  
The 54<sup>th</sup> Annual Symposium of the Vacuum Society of Japan  
(26-28/11/2013, International Congress Center EPOCHAL, Tsukuba, Japan)
6. “*DFT+U investigation on the adsorption and dissociation of oxygen on Pt-coated Ceria*”  
The 53<sup>rd</sup> Annual Symposium of the Vacuum Society of Japan  
(14-16/11/2012, Konan University, Kobe, Japan)
7. “*O<sub>2</sub> adsorption and dissociation on CeO<sub>2</sub>-supported Pt nanoparticles: A DFT+U study*”  
The 5<sup>th</sup> International Symposium on Atomically Controlled Fabrication Technology



- (22-24/10/2012, Osaka University, Osaka, Japan)
8. “*Spin effects in metal surface reactions: O<sub>2</sub> on ferromagnetic Pt*”  
AVS 58<sup>th</sup> International Symposium & Exhibition  
(30/10-04/11/2011, Nashville Convention Center, Nashville, Tennessee, USA)
  9. “*Oxygen dissociation on metal oxide-supported Pt cluster*”  
The 4<sup>th</sup> International Symposium on Atomically Controlled Fabrication Technology  
(31/10-02/11/2011, Osaka University, Osaka, Japan)
  10. “*Oxygen dissociative adsorption on Pt<sub>4</sub>/CeO<sub>2</sub>(111) surface*”  
The First JSMS Symposium on Multiscale Materials Modeling  
(23-24/05/2011, Osaka University, Osaka, Japan)
  11. “*Adsorption of nitric oxide on various metal phthalocyanines films by first-principles study*”  
The 3<sup>rd</sup> International Symposium on Atomically Controlled Fabrication Technology  
(24-26/11/2010, Osaka University, Osaka, Japan)
  12. “*Theoretical study on the oxygen vacancy formation in different platinum-coated CeO<sub>2</sub> surfaces of diesel oxidation catalysts*”  
The 27<sup>th</sup> European Conference on Surface Science  
(29/08-03/09/2010, Martiniplaza, Groningen, Kingdom of The Netherlands)
  13. “*Theoretical study on the adsorption of NO on metal phthalocyanines for biosensor application*”  
International Conference on Core Research and Engineering Science of Advanced Materials & Third International Conference on Nanospintronics Design and Realization  
(30/05-04/06/2010, Osaka University, Osaka, Japan)
  14. “*DFT study of oxygen vacancy formation in a diesel oxidation catalyst: Pt/CeO<sub>2</sub>(111)*”  
AVS 56<sup>th</sup> International Symposium & Exhibition  
(08-13/11/2009, San Jose Convention Center, San Jose, California, USA)
  15. “*A DFT study on adsorption of NO on various functional molecular nanowires*”  
Japanese Physical Society Meeting  
(25-28/09/2009, Kumamoto University, Kumamoto, Japan)
  16. “*Theoretical study on interaction of NO with metal tape-porphyrins*”  
First International Symposium on Atomically Controlled Fabrication Technology  
(16-17/02/2009, Osaka University, Osaka, Japan)
  17. “*DFT study on the adsorption of NO on various metal tape-porphyrins*”  
International Symposium on Surface Science and Nanotechnology  
(09-13/11/2008, Waseda University, Tokyo, Japan)
  18. “*Adsorption of NO on various metal tape-porphyrins by first-principles study*”  
International Conference on Quantum Simulators and Design 2008  
(31/05-03/06/2008, National Museum of Emerging Science and Innovation, Tokyo, Japan)
  19. “*The adsorption of diatomic molecules on iron tape-porphyrin: A comparative study*”  
International 21<sup>st</sup> Century COE Symposium on Atomistic Fabrication Technology 2007  
(15-17/10/2007, Osaka University, Osaka, Japan)
  20. “*A theoretical study on the interaction between iron tape-porphyrin and CO, NO, and O<sub>2</sub>*”  
Handai Nanoscience and Nanotechnology International Symposium  
(26-28/09/2007, Osaka University, Osaka, Japan)
  21. “*DFT study of Jahn-Teller effect in BaTiO<sub>3</sub>*”  
The 3<sup>rd</sup> International Workshop on Nanophysics and Nanotechnology  
(06-09/12/2006, Ha-Long, Vietnam)
  22. “*Calculation of electronic properties of BaTiO<sub>3</sub> using DFT method*”  
HUS Scientific Conference  
(11/11/2006, Ha-Noi University of Science, Ha-Noi, Vietnam)
  23. “*First-principles calculation for BaTiO<sub>3</sub>*”  
The 31<sup>st</sup> National Conference on Theoretical Physics  
(22-25/08/2006, Hon-Ngu Hotel, Cua-Lo, Nghe-An, Vietnam)

## OTHER RESEARCH AND EDUCATION RELATED ACTIVITIES

### Long-term Stay Research:

**Location:** Prof. Tetsuo Mohri's Group, Institute for Materials Science, Tohoku University

**Periods of stays:** ●14-28/01/2020 (2 weeks) ●30/09-11/10/2019 (2 weeks) ●03-14/12/2018 (2 weeks) ●04-15/06/2018 (2 weeks) ●24/07-04/08/2017 (2 weeks) ●16/01-30/01/2017 (2 weeks)

**Research topic:** Cluster expansion/variation methods and their applications for studying multi-component alloys (iron-carbon alloy, high-entropy alloys)

### Dissertation Supervision:

- 2018 - 2019:

Number of student: 1                      Status: Completed  
Academic degree: Master of Engineering  
Thesis title: “Atomistically kinematic simulations of carbon diffusion in  $\alpha$ -iron with point defects”

• **2017 - 2018:**

Number of student: 1                      Status: Completed  
Academic degree: Master of Engineering  
Thesis title: “Computational kinetics on diffusion process of carbon in iron bulk”

**Organizer/Co-organizer:**

- The 9<sup>th</sup> Asia CMD Workshop, Vietnam-Japan University, Hanoi, Vietnam (29/11-01/12/2017)
- The 5<sup>th</sup> Asia CMD Workshop, Hanoi University of Science, Hanoi, Vietnam (05-07/12/2013)
- The 4<sup>th</sup> Asia CMD Workshop, Hanoi University of Science, Hanoi, Vietnam (06-08/12/2012)
- HUS-OU-UBC International Workshop on Quantum Design and Realization, Osaka University, Osaka, Japan (27-28/02/2012)
- The 3<sup>rd</sup> Asia CMD Workshop, Saigon University, Ho Chi Minh City, Vietnam (09-11/12/2011)
- The 1<sup>st</sup> Asia CMD Workshop, Mahidol University, Bangkok, Thailand (15-17/02/2011)
- The 2<sup>nd</sup> Asia CMD Workshop, Hue University, Hue, Vietnam (16-18/12/2010)
- HUS-OU-BBK Scientific Workshop, Osaka University, Japan (22/11/2010)
- The 1<sup>st</sup> Asia CMD Workshop, Hanoi University of Science, Hanoi, Vietnam (16-18/12/2009)
- HUS-OU International Workshop on Quantum Simulation, Osaka University, Osaka, Japan (12/09/2008)
- HUS-OU International Workshop on Quantum Simulation, Osaka University, Osaka, Japan (13/09/2007)

**Journal Refereeing:**

- American Physical Society (Physical Review B)
- American Chemical Society (Journal of the American Chemical Society, Journal of Physical Chemistry)
- Elsevier (Chemical Physics, Chemical Physics Letter, Physica B: Condensed Matter, Solid State Communications)
- Institute of Physics, UK (Journal of Physics: Condensed Matter)
- Royal Society of Chemistry, UK (Physical Chemistry Chemical Physics)
- Physical Society of Japan (Journal of the Physical Society of Japan)
- Asia Pacific Higher Education Research Journal

**Memberships:**

- Japan Institute of Metals and Materials (present)
- American Physical Society (present)
- Materials Research Society (past)
- American Vacuum Society (past)
- Vietnam Theoretical Physics Society

**Others:**

- Supporter/Teaching Assistant for Vietnam-Japan University remote lectures
- Tutor for Asia CMD Workshop (Vietnam, Thailand, Philippines)
- Research supervisions/guidance for younger students in the group
- Setting up computational facilities for Asia CMD Workshop (Vietnam, Thailand)
- Research group's computer cluster system management
- Quantum Engineering Design Course official website establishment and maintenance

## COMPUTER SKILLS AND OUTPUTS

**Skills:**

- Operating systems: Windows, Mac OS X, Linux (Fedora, Ubuntu, SuSE, CentOS)
- Programming languages: Very experienced in FORTRAN, MATLAB; knowledgeable in C/C++, Python, MPI, Shell-scripts, Mathematica, HTML, Markdown, LaTeX
- Office applications: Microsoft Office, Apple iWork, OpenOffice
- Simulation packages: VASP, STATE-Senri, AkaiKKR, LAMMPS
- Visualization softwares: GNUplot, Matplotlib, VESTA, CrystalMaker, Ovito, AtomEye

**Outputs:**

- FORTRAN program for kinetic Monte-Carlo simulation of carbon diffusion and clustering in BCC iron
- FORTRAN program for calculating vibrational frequencies using Finite Difference Method
- FORTRAN program for calculating effective cluster interaction energies using Cluster Expansion Method
- FORTRAN program for calculating cluster probabilities of HEAs using Cluster Variation Method
- FORTRAN program for building Tersoff potentials for binary/ternary system using Genetic Algorithm

- FORTRAN program for building EAM potentials for ternary systems using Genetic Algorithm
- FORTRAN program for Monte Carlo simulation of magnetic properties of bimetallic surfaces
- FORTRAN utilities for analysis/manipulating output data of VASP and LAMMPS
- MATLAB Graphic User Interface program for Visualizing Hydrogen Atomic Orbitals