

CURRICULUM VITAE

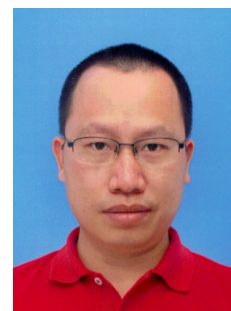
NGUYEN TIEN QUANG

Affiliation:

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Graduate School of Engineering
Division of Materials and Manufacturing Science
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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 •Seebeck coefficient
•Multi-Scale Modelling •First-Principles Calculation •Molecular Dynamics •Monte Carlo/Kinetic Monte Carlo
•Cluster Expansion/Variation Method •Evolutionary Algorithm •Interatomic Potential Development

PERSONAL DETAILS

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

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

- **04/2020 - present: Osaka University (Graduate School of Engineering)**

Position: Specially-Appointed Assistant Professor (full-time)
Main Duties: Doing research on Thermoelectric Materials (CREST Project)

- **12/2015 - 03/2020: Osaka University (Institute for NanoScience Design)**
(Professional development Consortium for Computational Materials Scientists)
Position: Specially-Appointed Assistant Professor (full-time)
Main 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)
Main Duties: Doing research on Hydrogen Behavior in Iron/Steel (ISMA Project)
- **10/2013 - 11/2013: Osaka University (Graduate School of Engineering)**
Position: Postdoctoral Researcher (part-time)
Main Duties: Doing research on Diesel Oxidation Catalysts
- **01/2008 - 09/2008: Osaka University (Graduate School of Engineering)**
Position: Specially-Appointed Researcher (full-time)
Main 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)
Main 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: O₂ on ferromagnetic Pt/M*” at the 54th 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 γ -Al₂O₃(111) surface*” at the 4th 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 Valmoria, 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”
Materials Transactions (*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 **316** (2020) 113918
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 **511** (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 α -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 O₂ on anatase TiO₂(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 CeO₂-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 γ -Al₂O₃(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 BaTiO₃"
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 α -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)
4. 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)

Manuscripts in Preparation:

1. Tien Quang Nguyen, Kazunori Sato and Yoji Shibutani
“*Kinetic Monte Carlo study on the diffusion properties and clustering of carbon in Fe-C alloy*”
To be submitted to Modelling and Simulation in Materials Science and Engineering
2. Tien Quang Nguyen, Kazunori Sato and Yoji Shibutani
“*Effects of low carbon content on the tetragonality of iron lattice*”
To be submitted to Materials Transactions
3. Tien Quang Nguyen, Mary Clare Sison Escano and Hideaki Kasai
“*DFT+U study on the adsorption and oxidation of NO on O-precovered Pt₄/CeO₂*”
To be submitted to Applied Surface Science
4. Tien Quang Nguyen, Hajime Kimizuka and Shigenobu Ogata
“*Development of an interatomic potential for the Fe-C-H ternary alloy*”
To be submitted to Physical Review B
5. Tien Quang Nguyen, Hajime Kimizuka and Shigenobu Ogata
“*Hydrogen-vacancy-carbon formation in bcc iron: First-principles investigation*”
To be submitted to ISIJ International

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:

1. “*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)
2. “*Atomistically kinetic simulations of carbon behavior in bcc iron with point defect*”
Short-talk Session at the 35th Computational Materials Design
(02-06/09/2019, Osaka University, Osaka, Japan)
3. “*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)
4. “*Computational kinetics on diffusion of carbons in bcc iron*”
Scientific Seminar at Institute for Materials Research
(07/06/2018, Tohoku University, Miyagi, Japan)
5. “*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)
6. “*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)
7. “*Interatomic potentials development of Fe-C binary system for atomistic materials design of new heterogeneous iron*”
Scientific Seminar at Faculty of Physics
(04/11/2016, Hanoi National University of Education, Hanoi, Vietnam)
8. “*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)
9. *"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)
 10. *"Computational Materials Design for energy and environmental applications"*
Scientific Seminar at Faculty of Physics
(06-08/12/2012, VNU University of Science, Hanoi, Vietnam)
 11. *"Porphyrins and macrocycles: From basics to applications"*
ECS 221st Meeting
(06-10/05/2012, Washington State Convention Center, Seattle, Washington, USA)

Lectures for Graduate Students:

1. *"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)
2. *"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)
3. *"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)
4. *"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. *"Cluster variation calculations of pair probabilities in multicomponent alloy: Application to the fcc Cr-Fe-Mn-Ni system"*
The 166th Annual Spring Meeting of the Japan Institute of Metals and Materials
(17-19/03/2020, Tokyo Institute of Technology, Tokyo, Japan)
2. *"Atomistic kinematics of carbon diffusion and clustering in bcc Fe with point defects"*
APS March Meeting 2020
(02-06/03/2020, Colorado Convention Center, Denver, Colorado, USA)
3. *"Carbon diffusion and clustering in bcc iron: A kinetic Monte Carlo study"*
Workshop on Nanotechnology-Driven Topics
(10/12/2019, Osaka University, Osaka, Japan)
4. *"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)
5. *"Atomistically kinetic simulations of carbon diffusion in α -Fe with point defect"*
The 32nd Meeting on Computational Mechanics of the Japan Society of Mechanical Engineers
(16-18/09/2019, Toyo University, Saitama, Japan)
6. *"Cluster Expansion simulations of Fe-C alloys with point defects: Atomic and effective cluster interactions"*
The 164th Annual Spring Meeting of the Japan Institute of Metals and Materials
(20-22/03/2019, Tokyo Denki University, Tokyo, Japan)
7. *"Diffusion properties of carbon in Fe-C alloy using new Tersoff potential"*
The 31st Meeting on Computational Mechanics of the Japan Society of Mechanical Engineers
(23-25/11/2018, Tokushima University, Tokushima, Japan)
8. *"Diffusion properties of carbon in α -Fe"*
PCoMS Symposium & Annual Meeting of Supercomputing Consortium for Computational Materials Science 2018
(22-23/10/2018, Tohoku University, Miyagi, Japan)
9. *"Cluster Expansion Method study on the effective interaction in Fe-C alloys"*
The 163rd Annual Fall Meeting of the Japan Institute of Metals and Materials
(19-21/09/2018, Tohoku University, Miyagi, Japan)
10. *"Construction of interatomic potential for Fe-C systems using evolutionary algorithm"*
APS March Meeting 2018
(05-09/03/2018, Los Angeles Convention Center, Los Angeles, California, USA)
11. *"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)
12. *"New atomic potential of Fe-C binary system for phase transformation of heterogeneous materials"*
The 161th Annual Fall Meeting of the Japan Institute of Metals and Materials
(06-08/09/2017, Hokkaido University, Hokkaido, Japan)
 13. *"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)
 14. *"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)
 15. *"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)
 16. *"NO oxidation on CeO₂-supported Pt₄ cluster: A DFT+U study"*
Quantum Engineering Design Workshop
(25/10/2013, Osaka University, Osaka, Japan)
 17. *"NO oxidation on O pre-covered Pt₄/CeO₂"*
OU-TUM Workshop: Trends in Catalysis
(16/05/2013, Osaka University, Osaka, Japan)
 18. *"Theoretical Investigation on NO oxidation on O pre-covered Pt₄/CeO₂"*
International Workshop on the Theory of Dense Kondo Systems
(19-20/03/2013, Osaka University, Osaka, Japan)
 19. *"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)
 20. *"Oxidation of metal and metal oxide systems"*
Asia Computational Materials Design Workshop
(10-12/10/2011, De La Salle University, Manila, Philippines)
 21. *"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)
 22. *"First-principles study on nitric oxide adsorption on metal tape-porphyrines"*
Asia Computational Materials Design Workshop
(15-17/02/2011, Mahidol University, Bangkok, Thailand)
 23. *"Adsorption of nitric oxide on metal porphyrin tape"*
Asia Computational Materials Design Workshop
(16-18/12/2010, Hue University, Hue, Vietnam)
 24. *"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)
 25. *"Nitric oxide adsorption effects on metal phthalocyanines"*
OU-DLSU Academic Research Workshop
(27-28/05/2010, Osaka University, Osaka, Japan)
 26. *"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)
 27. *"NO adsorption effects on metal tape-porphyrins"*
GCOE International Workshop
(25-27/11/2008, Osaka University, Osaka, Japan)
 28. *"The adsorption of NO on various metal tape-porphyrins"*
ITB-OU Academic Research Workshop
(30/06/2008, Osaka University, Osaka, Japan)
 29. *"DFT study on the binding of CO, NO, and O₂ to iron tape-porphyrin"*
International Workshop on Quantum Simulation 2007
(13/09/2007, Osaka University, Osaka, Japan)

30. "*O₂ adsorption effects on electronic properties of Fe tape-porphyrin*"
International Science and Engineering Workshop
(15/05/2007, Osaka University, Osaka, Japan)
31. "*DFT study on O₂ adsorbed Fe tape-porphyrin*"
The 3rd International Workshop on Reactions Involving Oxygen
(10/05/2007, Osaka University, Osaka, Japan)
32. "*Study of electronic properties of perovskite BaTiO₃*"
The 4th 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 α -Fe in the presence of vacancy*"
The 22th 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 α -iron*"
The 9th 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 9th 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_n/CeO₂(111)*"
The 54th 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 53rd Annual Symposium of the Vacuum Society of Japan
(14-16/11/2012, Konan University, Kobe, Japan)
7. "*O₂ adsorption and dissociation on CeO₂-supported Pt nanoparticles: A DFT+U study*"
The 5th International Symposium on Atomically Controlled Fabrication Technology
(22-24/10/2012, Osaka University, Osaka, Japan)
8. "*Spin effects in metal surface reactions: O₂ on ferromagnetic Pt*"
AVS 58th International Symposium & Exhibition
(30/10-04/11/2011, Nashville Convention Center, Nashville, Tennessee, USA)
9. "*Oxygen dissociation on metal oxide-supported Pt cluster*"
The 4th International Symposium on Atomically Controlled Fabrication Technology
(31/10-02/11/2011, Osaka University, Osaka, Japan)
10. "*Oxygen dissociative adsorption on Pt₄/CeO₂(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 3rd 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 CeO₂ surfaces of diesel oxidation catalysts*"
The 27th 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/CeO₂(111)*"
AVS 56th 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 21st 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 O₂*”
Handai Nanoscience and Nanotechnology International Symposium
(26-28/09/2007, Osaka University, Osaka, Japan)
 21. “*DFT study of Jahn-Teller effect in BaTiO₃*”
The 3rd International Workshop on Nanophysics and Nanotechnology
(06-09/12/2006, Ha-Long, Vietnam)
 22. “*Calculation of electronic properties of BaTiO₃ using DFT method*”
HUS Scientific Conference
(11/11/2006, Ha-Noi University of Science, Ha-Noi, Vietnam)
 23. “*First-principles calculation for BaTiO₃*”
The 31st 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 α -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 9th Asia CMD Workshop, Vietnam-Japan University, Hanoi, Vietnam (29/11-01/12/2017)
- The 5th Asia CMD Workshop, Hanoi University of Science, Hanoi, Vietnam (05-07/12/2013)
- The 4th 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 3rd Asia CMD Workshop, Saigon University, Ho Chi Minh City, Vietnam (09-11/12/2011)
- The 1st Asia CMD Workshop, Mahidol University, Bangkok, Thailand (15-17/02/2011)
- The 2nd Asia CMD Workshop, Hue University, Hue, Vietnam (16-18/12/2010)
- HUS-OU-BBK Scientific Workshop, Osaka University, Japan (22/11/2010)
- The 1st 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, Phonopy
- 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

Last update: May 06, 2020