CURRICULUM VITAE

NGUYEN TIEN QUANG

Affiliation:
Osaka University
Institute for NanoScience Design
1-3 Machikaneyama-cho, Toyonaka-shi, Osaka 560-8531, JAPAN

Contact Information:
Telephone: (81) 06 6105 5884 | **Mobile:** (81) 080 4240 1906
E-mail: quang@insd.osaka-u.ac.jp | **Website:** https://ntq1982.github.io

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
- **Nationality:** Vietnam
- **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

- **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 Si_xGe_{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_2 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-Al_2O_3(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*"
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 **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 a-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_2 on anatase TiO_2(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_2-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-Al_2O_3(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 $BaTiO_3$*"
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)

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 heterogenous 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. "*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 a-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)
4. "*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)
5. "*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)
6. "*Diffusion properties of carbon in a-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 163rd 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 161th 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_2-supported Pt_4 cluster: A DFT+U study*"
    Quantum Engineering Design Workshop
    (25/10/2013, Osaka University, Osaka, Japan)
15. "*NO oxidation on O pre-covered Pt_4/CeO_2*"
    OU-TUM Workshop: Trends in Catalysis
    (16/05/2013, Osaka University, Osaka, Japan)
16. "*Theoretical Investigation on NO oxidation on O pre-covered Pt_4/CeO_2*"
    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_2 to iron tape-porphyrin*"
    International Workshop on Quantum Simulation 2007
    (13/09/2007, Osaka University, Osaka, Japan)
28. "*O_2 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_2 adsorbed Fe tape-porphyrin*"
    The 3rd International Workshop on Reactions Involving Oxygen
    (10/05/2007, Osaka University, Osaka, Japan)
30. "*Study of electronic properties of perovskite $BaTiO_3$*"
    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 $Pt_n/CeO_2(111)$*"
   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. "*O_2 adsorption and dissociation on CeO_2-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: O_2 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 $Pt_4/CeO_2(111)$ 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 CeO_2 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: $Pt/CeO_2(111)$*"
    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 O_2*"
    Handai Nanoscience and Nanotechnology International Symposium
    (26-28/09/2007, Osaka University, Osaka, Japan)
21. "*DFT study of Jahn-Teller effect in $BaTiO_3$*"
    The 3rd International Workshop on Nanophysics and Nanotechnology
    (06-09/12/2006, Ha-Long, Vietnam)
22. "*Calculation of electronic properties of $BaTiO_3$ using DFT method*"
    HUS Scientific Conference
    (11/11/2006, Ha-Noi University of Science, Ha-Noi, Vietnam)
23. "*First-principles calculation for $BaTiO_3$*"
    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)
- Programing languages: Very experienced in FORTRAN, MATLAB; knowledgable 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

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