

CURRICULUM VITAE

NGUYEN TIEN QUANG

Current Position:

Assistant Professor (full-time) at Osaka University
Lecturer (part-time) at Vietnam-Japan University

Affiliations:

- (1) **Institute for NanoScience Design**
Osaka University
1-3 Machikaneyama-cho, Toyonaka-shi, Osaka 560-8531, JAPAN
- (2) **Center for Open Innovation Research and Education**
Graduate School of Engineering, Osaka University
2-1 Yamadaoka, Suita-shi, Osaka 565-0871, JAPAN
- (3) **Master Program in Nanotechnology**
Vietnam-Japan University
Luu Huu Phuoc Road, My Dinh 1 Ward, Nam Tu Liem District, Ha Noi, VIETNAM



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Research Fields:

Computational Physics/Chemistry, Computational Materials Science, Condensed Matter Physics

PERSONAL DETAILS

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

ACADEMIC QUALIFICATIONS

- **10/2010 - 09/2013: Osaka University (Graduate School of Engineering)**
Quantum Engineering Design Program
Degree and Major: Doctor of Philosophy in Engineering
Thesis Title: Theoretical Study on Nitric Oxide Adsorption and Oxidation on Metallo-Macrocycles and Ceria-Supported Platinum Cluster
- **10/2008 - 09/2010: Osaka University (Graduate School of Engineering)**
Quantum Engineering Design Program
Degree and Major: Master of Engineering
Thesis Title: Adsorption of Nitric Oxide on Metal Porphyrin Tape: The Role of Metal Porphyrin Tape as Sensor in Detecting Nitric Oxide Gas
- **12/2004 - 12/2006: Vietnam National University, Hanoi (Graduate School of Science)**
Degree and Major: Master of Science in Theoretical Physics
Thesis Title: DFT Study on The Electronic Properties of Perovskite
- **09/2000 - 06/2004: Vietnam National University, Hanoi (School of Science)**
Teacher Licensure Program
Degree and Major: Bachelor of Science in Physics/Physics Education
Thesis Title: Quantum Visualization of Hydrogen Atom

TEACHING EXPERIENCE

- **10/2017 - 08/2019: Master Program in Nanotechnology, Vietnam-Japan University**
Location: Hanoi, Vietnam
Position: Lecturer (part-time)
Duties: Teaching master course students and supervising student's thesis
- **05/2017 - 06/2017: Master Program in Nanotechnology, Vietnam-Japan University**
Location: Hanoi, Vietnam
Position: Lecturer (part-time)
Duties: Teaching master course students

WORK EXPERIENCE

- **12/2015 - present: Institute for NanoScience Design, Osaka University**
(under Professional Development Consortium for Computational Materials Scientists)
Location: Osaka, Japan
Position: Assistant Professor (full-time)
Duties: Doing research on Atomistic Materials Design of New Heterogeneous Iron/Steel
- **12/2013 - 12/2015: Graduate School of Engineering Science, Osaka University**
Location: Osaka, Japan
Position: Postdoctoral Researcher (full-time)
Duties: Doing research on Hydrogen Behavior in Iron/Steel
- **10/2013 - 11/2013: Graduate School of Engineering, Osaka University**
Location: Osaka, Japan
Position: Postdoctoral Researcher (full-time)
Duties: Doing research on Diesel Oxidation Catalysts (DOCs) and Three-Way Catalysts (TWCs)
- **01/2008 - 09/2008: Graduate School of Engineering, Osaka University**
Location: Osaka, Japan
Position: Special Researcher (full-time)
Duties: Doing research on Molecular Devices (gas sensors) and Diesel Oxidation Catalysts (DOCs)
- **01/2007 - 12/2007: Graduate School of Engineering, Osaka University**
Location: Osaka, Japan
Position: Special Researcher (full-time)
Duties: Doing research on Molecular Devices (gas sensors) and Fuel Cell
- **06/2004 - 12/2006: Graduate School/School of Science, Vietnam National University, Hanoi**
Location: Hanoi, Vietnam
Position: Teaching Assistant (part-time)
Duties: Instruction for undergraduate students on MATLAB practice tutorials

RESEARCH FIELDS OR SPECIALIZATION

- **Atomistic Materials Design of New Heterogeneous Iron/Steel:**
Study of the phase transformation of iron between ferrite and martensite phases, the formation of cementite in steel and the effect of solute atoms (carbon, nitrogen, boron,...) on the mechanical properties of iron/steel for various industrial applications by using phase-field modeling, first-principles and molecular dynamics methods
- **Hydrogen Behavior in Iron/Steel:**
Study of the hydrogen interaction with various defects (vacancies, dislocation, grain boundaries,...) and solutes (carbon, nitrogen, sulfur,...) in iron; and the effects of hydrogen on the mechanical properties of iron/steel for various industrial applications by using first-principles and molecular dynamics methods
- **Diesel Oxidation Catalysts, Three-Way Catalysts:**
Study of oxidation/reduction processes of gases on metal surfaces and metal oxide supported metal clusters for heterogeneous catalysis applications by using DFT+U and 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 oxidation processes on bimetallic surfaces for renewable energy applications by using first-principles and Monte Carlo methods

INDUSTRIAL RESEARCH EXPERIENCE

- CREST Project: Thermal Control (2019 - present)
- ISMA (NEDO) Project: Hydrogen Behavior in Iron/Steel (2013 - 2015)
- TANAKA Precious Metals Group Project: Cathode Catalysts for Fuel Cell (2013)
- ISUZU Motor Inc. Project: Diesel Oxidation Catalyst for Automobile (2008 - 2013)
- SHARP Corporation Project: Molecular Devices for Gas Sensors (2007 - 2009)

PATENT

Title: 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

Patent Number: JP2011080798-A

Inventor(s): T. Q. NGUYEN, M. OTONASHI, T. KAWATA, M. YAMANAKA, K. HARA, H. KASAI, H. NAKANISHI

Patent Assignee Name(s) and Code(s): SHARP KK(SHAF-C)

Derwent Primary Accession Number: 2011-E14890 [35]

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)

ACQUISITION OF FUNDS

Japan GCOE (Global Center of Excellence TEAM Program):

- Tien Quang Nguyen (Team Leader), Ferensa Oemry, Saputro Adhitya Gandaryus, Koji Shimizu, Chong Kong Ng. "A Theoretical Study of dynamics and characteristics of oxygen reduction reaction for new catalyst development" (2012-2013)
- Tien Quang Nguyen (Team Leader), Aspera Susan Meñez, Wungu Triati Dewi Kencana, Moreno Joaquin Lorenzo Valmoria, Saputro Adhitya Gandaryus, Yohei Ushijima. "The theoretical analysis on the application to electronic devices using organic materials" (2011-2012)
- Tien Quang Nguyen (Team Leader), Hirofumi Kishi, Mary Clare Sison Escano, Abdulla Ali Abdulla Sarhan, Ferensa Oemry. "Design of thin film nano-devices using simulation technology" (2009-2010)

PUBLICATIONS

Book chapters:

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

Journals:

1. Tien Quang Nguyen, Hajime Kimizuka, Shigenobu Ogata, "Development of an interatomic potential for the Fe-C-H system", Physical Review B (status: manuscript in preparation)
2. Tien Quang Nguyen, Hajime Kimizuka, Shigenobu Ogata, "Hydrogen-vacancy-carbon formation in BCC iron: First-principles investigation", Computational Materials Science (status: manuscript in preparation)
3. Tien Quang Nguyen, Mary Clare Sison Escano, Kazunori Sato, Yoji Shibutani, Tamio Oguchi, Tetsuo Mohri, "Cluster expansion method study on the effective cluster interactions in FeC alloys", ISIJ International (status: submitted for review)
4. Mary Clare Sison Escano, Tien Quang Nguyen, Yu Osanai, Hideaki Kasai, Masahiko Tani, "Large-scale spin-polarized DFT calculation of electronic properties of GaAs with defects", Materials Research Express, 6 (2019) 055914

5. Tien Quang Nguyen, Kazunori Sato, Yoji Shibutani, "Development of Fe-C interatomic potential for carbon impurities in α -iron", *Computational Materials Science*, 150 (2018) 510
6. Tien Quang Nguyen, Kazunori Sato, Yoji Shibutani, "First-principles study of the BCC/FCC phase transition promoted by interstitial carbon in iron", *Materials Transactions*, 59 (2018) 870
7. Mary Clare Sison Escano, Tien Quang Nguyen, Hideaki Kasai, "Spin-up "pristine-like" Dirac cone in bridge-structure graphene on Ni(111)", *Applied Surface Science*, 427 (2018) 949
8. Mary Clare Sison Escano, Tien Quang Nguyen, Hideaki Kasai, "Another way of looking at reactivity enhancement in large area graphene: The role of exchange-splitting from first-principles methods", *The Journal of Physical Chemistry C*, 119 (2015) 26636
9. Nguyen Hoang Linh, Tien Quang Nguyen, Wilson Agerico Dino, Hideaki Kasai, "Effect of oxygen vacancy on the adsorption of O₂ on anatase TiO₂(001): A DFT-based study", *Surface Science*, 633 (2015) 38
10. Tien Quang Nguyen, Mary Clare Sison Escano, Hiroshi Nakanishi, Hideaki Kasai, Hiroyoshi Maekawa, Kazuo Osumi, Kaoru Sato, "DFT+U study on the oxygen adsorption and dissociation on CeO₂-supported platinum cluster", *Applied Surface Science*, 288 (2014) 244
11. Tien Quang Nguyen, Allan Abraham Bustria Padama, Mary Clare Sison Escano, Hideaki Kasai, "Theoretical study on The adsorption of NO on metal macrocycles, Metal=Mn,Fe,Co,Ni,Cu,Zn", *ECS Transactions*, 45 (2013) 91
12. Mary Clare Sison Escano, Tien Quang Nguyen, Hideaki Kasai, "Molecular oxygen adsorption on ferromagnetic platinum", *Chemical Physics Letters*, 555 (2013) 125
13. Hirofumi Kishi, Ferensa Oemry, Tien Quang Nguyen, Shinichi Kunikata, Hiroshi Nakanishi, Hideaki Kasai, Hiroyoshi Maekawa, Kazuo Osumi, "Study of NO oxidation reaction over the Pt cluster supported on γ -Al₂O₃(111) surface", *Current Applied Physics*, 12 (2012) S110
14. Mary Clare Sison Escano, Tien Quang Nguyen, Hideaki Kasai, "Analysis of band gap formation in graphene by Si impurities: Local bonding interaction rules", *Chemical Physics Letters*, 515 (2011) 85
15. Mary Clare Sison Escano, Tien Quang Nguyen, Hideaki Kasai, "Molecular and electronic tuning of Si/CNT hybrid system", *Japanese Journal of Applied Physics*, 50 (2011) 045101
16. Tien Quang Nguyen, Mary Clare Sison Escano, Hideaki Kasai, "Nitric oxide adsorption effects on metal phthalocyanines", *Journal of Physical Chemistry B*, 114 (2010) 10017
17. Mary Clare Sison Escano, Tien Quang Nguyen, Hiroshi Nakanishi, 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
18. Tien Quang Nguyen, Susan Menez Aspera, Hiroshi Nakanishi, Hideaki Kasai, "NO adsorption effects on various functional molecular nanowires", *Computational Materials Science*, 47 (2009) 111
19. Tien Quang Nguyen, Mary Clare Sison Escano, Reiko Tanaka, Hiroshi Nakanishi, 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
20. Mary Clare Sison Escano, Tien Quang Nguyen, Hiroshi Nakanishi, Hideaki Kasai, "Bonding of Pt/Fe overlayer and its effects on atomic oxygen chemisorption from density functional theory study", *Surface Science*, 602 (2008) 3415
21. Tien Quang Nguyen, Mary Clare Sison Escano, Nobuaki Shimoji, Hiroshi Nakanishi, Hideaki Kasai, "Adsorption of diatomic molecules on iron tape-porphyrin: A comparative study", *Physical Review B*, 77 (2008) 195307
22. Tien Quang Nguyen, Mary Clare Sison Escano, Nobuaki Shimoji, Hiroshi Nakanishi, Hideaki Kasai, "DFT study on the adsorption of NO on iron tape-porphyrin", *Surface and Interface Analysis*, 40 (2008) 1082

Proceedings:

1. Tien Quang Nguyen, Ngoc Nam Ho, Thi Thu Dinh Ngo, Kazunori Sato, Yoji Shibutani, "Diffusion properties of carbon in Fe-C alloy using new Tersoff potential", 日本機械学会 第31回計算力学講演会 (CMD2018) CD-ROM
2. Mary Clare Sison Escano, Tien Quang Nguyen, Hiroshi Nakanishi, Hideaki Kasai, "Controlling oxidation reaction on platinum by spin manipulation", *Nanotechnology 2012: Electronics, Devices, Fabrication, MEMS, Fluidics and Computational Volume 2*, Chapter 9: Modeling and Simulation at the Nanoscale, USA (2012) 645-648, ISBN: 978-1-4665-6275-2
3. Tien Quang Nguyen and Thanh Cong Bach, "First-principles calculation for BaTiO₃", *Communications in Physics*, 17 (2007) 128

PRESENTATIONS

Lectures:

1. "Nanomechanics: Introduction on Molecular Dynamics simulation" - Lecture for master course students in Nanotechnology Program, VJU (20-27/12/2018, Vietnam Japan University, Hanoi, Vietnam)

2. “Nanomechanics: Introduction on Molecular Dynamics simulation” - Lecture for master course students in Nanotechnology Program, VJU (25/11-11/12/2017, Vietnam Japan University, Hanoi, Vietnam)
3. “Nanomechanics: Introduction on Molecular Dynamics simulation” - Lecture for master course students in Nanotechnology Program, VJU (08-22/05/2017, Vietnam Japan University, Hanoi, Vietnam)
4. “Interatomic potentials development of Fe-C binary system for atomistic materials design of new heterogeneous iron” - Lecture at Faculty of Physics, HNUE (04/11/2016, Hanoi National University of Education, Hanoi, Vietnam)
5. “Computational Materials Design for energy and environmental applications” - Lecture for undergraduate students at Faculty of Physics, HUS (06-08/12/2012, Hanoi University of Science, Hanoi, Vietnam)

Seminars:

1. “Diffusion properties of carbon and tetragonality effect in Fe-C alloy”, Scientific Seminar at Mohri Laboratory, Institute for Materials Research (06/12/2018, Tohoku University, Miyagi, Japan)
2. “Computational kinetics on diffusion of carbons in bcc iron”, Scientific Seminar at Mohri Laboratory, Institute for Materials Research (07/06/2018, Tohoku University, Miyagi, Japan)
3. “Atomistic materials design of new heterogeneous steel: Computational kinetics on diffusion of carbons in iron”, PCoMS Scientific Seminar, The Institute of Scientific and Industrial Research (15/05/2018, Osaka University, Osaka, Japan)
4. “Atomistic materials design of new steel with highly-tuned strength, ductility and fracture toughness: Development of Fe-C interatomic potential”, Scientific Seminar at Kakeshita Laboratory, Division of Materials Science and Engineering, Graduate School of Engineering (06/10/2017, Osaka University, Osaka, Japan)
5. “Analytic interatomic potential for modeling phase transformation in the Fe-C system”, Scientific Seminar at Mori Laboratory, 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 Kakeshita Laboratory, Division of Materials Science and Engineering, Graduate School of Engineering (14/04/2017, Osaka University, Osaka, Japan)
7. “Analytic bond-order potential for atomistic simulations of Fe-C system”, Scientific Seminar at Mori Laboratory, Center for Computational Materials Science, Institute for Materials Research (18/01/2017, Tohoku University, Miyagi, Japan)
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. “Hydrogen behaviors in steels: Hydrogen/carbon/vacancy interaction”, Scientific Seminar at Ogata Laboratory, Graduate School of Engineering Science (17/06/2015, Osaka University, Osaka, Japan)
10. “Uranium: The metal of tomorrow”, Nandemo Seminar at Kasai Laboratory, Graduate School of Engineering (15/11/2013, Osaka University, Osaka, Japan)
11. “NO oxidation on CeO₂-supported Pt₄ cluster”, Project Seminar at ISUZU Advanced Engineering Center (08/02/2013, Isuzu Motors Fujisawa Plant, Kanagawa, Japan)
12. “Nitric oxide adsorption on oxygen pre-covered Pt₄/CeO₂”, Project Seminar at ISUZU Advanced Engineering Center (13/07/2011, Isuzu Motors Fujisawa Plant, Kanagawa, Japan)

Oral (International Conferences):

1. “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)
2. “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)
3. “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)
4. “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)
5. “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)
6. “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)

7. "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)
8. "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)
9. "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)
10. "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)
11. "NO oxidation on CeO₂-supported Pt₄ cluster: A DFT+U study", Quantum Engineering Design Workshop (25/10/2013, Osaka University, Osaka, Japan)
12. "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) - **Invited talk**
13. "NO oxidation on O pre-covered Pt₄/CeO₂", OU-TUM Workshop: Trends in Catalysis (16/05/2013, Osaka University, Osaka, Japan)
14. "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)
15. "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)
16. "Porphyrins and macrocycles: From basics to applications", ECS 221st Meeting (06-10/05/2012, Washington State Convention Center, Seattle, Washington, USA) - **Invited talk**
17. "Oxidation of metal and metal oxide systems", Asia Computational Materials Design Workshop (10-12/10/2011, De La Salle University, Manila, Philippines)
18. "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)
19. "First-principles study on nitric oxide adsorption on metal tape-porphyrines", Asia Computational Materials Design Workshop (15-17/02/2011, Mahidol University, Bangkok, Thailand)
20. "Adsorption of nitric oxide on metal porphyrin tape", Asia Computational Materials Design Workshop (16-18/12/2010, Hue University, Hue, Vietnam)
21. "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)
22. "Nitric oxide adsorption effects on metal phthalocyanines", OU-DLSU Academic Research Workshop (27-28/05/2010, Osaka University, Osaka, Japan)
23. "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)
24. "NO adsorption effects on metal tape-porphyrins", GCOE International Workshop (25-27/11/2008, Osaka University, Osaka, Japan)
25. "The adsorption of NO on various metal tape-porphyrins", ITB-OU Academic Research Workshop (30/06/2008, Osaka University, Osaka, Japan)
26. "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)
27. "O₂ adsorption effects on electronic properties of Fe tape-porphyrin", International Science and Engineering Workshop (15/05/2007, Osaka University, Osaka, Japan)
28. "DFT study on O₂ adsorbed Fe tape-porphyrin", The 3rd International Workshop on Reactions Involving Oxygen (10/05/2007, Osaka University, Osaka, Japan)
29. "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 (International Conferences):

1. "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)
2. "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)

3. "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)
4. "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)
5. "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)
6. "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)
7. "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)
8. "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)
9. "Oxygen dissociative adsorption on Pt₄/CeO₂(111) surface", The First JSMS Symposium on Multiscale Materials Modeling (23-24/05/2011, Osaka University, Osaka, Japan)
10. "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)
11. "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)
12. "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)
13. "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)
14. "A DFT study on adsorption of NO on various functional molecular nanowires", Japanese Physical Society Meeting (25-28/09/2009, Kumamoto University, Kumamoto, Japan)
15. "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)
16. "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)
17. "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)
18. "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)
19. "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)
20. "DFT study of Jahn-Teller effect in BaTiO₃", The 3rd International Workshop on Nanophysics and Nanotechnology (06-09/12/2006, Ha-Long, Vietnam)
21. "Calculation of electronic properties of BaTiO₃ using DFT method", HUS Scientific Conference (11/11/2006, Ha-Noi University of Science, Ha-Noi, Vietnam)
22. "First-principles calculation for BaTiO₃", The 31st National Conference on Theoretical Physics (22-25/08/2006, Hon-Ngu Hotel, Cua-Lo, Nghe-An, Vietnam)

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: MS Office, Apple iWork, OpenOffice
- Simulation packages: Dacapo, VASP, STATE-Senri, AkaiKKR, LAMMPS
- Visualization softwares: GNUplot, Matplotlib, VESTA, CrystalMaker, VMD, Ovito, AtomEye

Outputs:

- FORTRAN program for Kinetic Monte-Carlo simulation of carbon diffusion and clustering in iron

- FORTRAN program for calculating vibrational frequencies using Finite Difference Method
- FORTRAN program for calculating interactive interaction energies using Cluster Expansion Method
- FORTRAN program for generating bond-order potentials for binary system using Genetic Algorithm
- FORTRAN program for generating interatomic 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 Vienna Ab-initio Simulation Program
- MATLAB Graphic User Interface program for Visualizing Hydrogen Atomic Orbitals

OUTREACH

Organizer of:

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

MEMBERSHIPS

- The American Physical Society (US)
- The Japan Institute of Metals and Materials (JP)
- The Materials Research Society (US)
- The Vacuum Society of Japan (JP)
- The Physical Society of Japan (JP)
- The American Vacuum Society (US)
- Vietnamese Theoretical Physical Society (VN)

JOURNAL REFEREEING

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

OTHERS

- Supporter/Teaching Assistant for Vietnam-Japan University remote lectures
- Tutor for Asia CMD Workshop (Vietnam, Thailand, Philippines)
- Research supervisions/guidance for younger students
- 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