CURRICULUM VITAE

NGUYEN TIEN QUANG

Current Affiliation:
Osaka University
Graduate School of Engineering
Division of Materials and Manufacturing Science
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Research IDs:
●**Scopus:** 36011850900 ●**ORCID:** 0000-0003-1148-2271 ●**J-GLOBAL:** 202101002092651300

Research Interests:
●Computational Physics/Chemistry ●Computational Materials Science ●Condensed Matter Physics ●Molecular Electronic Devices ●Fuel Cells ●Diesel Oxidation Catalysts ●Diffusion in Metals and Alloys ●Iron-Carbon Alloys ●High-Entropy Alloys ●Thermoelectric Materials ●Multi-Scale Modeling ●First-Principles Calculations ●Molecular Dynamics ●Monte Carlo/Kinetic Monte Carlo ●Cluster Expansion/Variation Method ●Phase-field Modelling ●Interatomic Potential Development ●Evolutionary Algorithms ●Artificial Neural Networks

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PERSONAL DETAILS

- **Full Name:** Tien Quang, NGUYEN
- **Gender:** Male
- **Nationality:** Vietnamese
- **Language Proficiency:** Vietnamese (native), English (fluent), Japanese (basic)

EDUCATIONAL HISTORY

- **2010/10 - 2013/09: 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

- **2008/10 - 2010/09: 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

- **2007/01 - 2007/12: Osaka University (Graduate School of Engineering)**
  JASSO Exchange Student Program
  Supervisor: Prof. Hideaki Kasai

- **2004/12 - 2006/12: Vietnam National University (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

- **2000/09 - 2004/08: Vietnam National University (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

- **2020/04 - present: Osaka University (Graduate School of Engineering)**
  Position: Specially-Appointed Assistant Professor (full-time)
  Main Duties: Doing research on Thermoelectric Materials and Impurities Behavior in Iron/Steel
  Other Duties: Teaching master course students at Vietnam-Japan University and co-supervising theses for doctor course students at Osaka University

- **2015/12 - 2020/03: Osaka University (Institute for NanoScience Design)**
  (Professional development Consortium for Computational Materials Scientists - PCoMS)
  Position: Specially-Appointed Assistant Professor (full-time)
  Main Duties: Doing research on Atomistic Materials Design of New Heterogeneous Iron/Steel
  Other Duties: Teaching and supervising theses for master course students at Vietnam-Japan University

- **2013/12 - 2015/12: Osaka University (Graduate School of Engineering Science)**
  Position: Postdoctoral Researcher (full-time)
  Main Duties: Doing research on Hydrogen Behavior in Iron/Steel

- **2013/10 - 2013/11: Osaka University (Graduate School of Engineering)**
  Position: Postdoctoral Researcher (part-time)
  Main Duties: Doing research on Fuel Cells and Diesel Oxidation Catalysts

- **2008/01 - 2008/09: Osaka University (Graduate School of Engineering)**
  Position: Specially-Appointed Researcher (full-time)
  Main Duties: Doing research on Molecular Electronic Devices and Diesel Oxidation Catalysts

- **2004/06 - 2006/12: Vietnam National University (Hanoi) (VNU University of Science)**
  Position: Teaching Assistant (part-time)
  Main Duties: Practice guidance on MATLAB and Mathematica for undergraduate/graduate students

TEACHING EXPERIENCE

- **2020/04 - present: Osaka University (Graduate School of Engineering)**
  Duties: Co-supervising doctor course students' theses

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

- **2004/06 - 2006/12: Vietnam National University (Hanoi) (VNU University of Science, Faculty of Physics)**
  Duties: Practice guidance on MATLAB and Mathematica for undergraduate/graduate students

RESEARCH EXPERIENCE

- **Thermoelectric Materials:** Investigation into the unusual behaviors in electron and lattice thermal conductivities of transition metal-doped semiconductors for improving the thermoelectric efficiency of thermoelectric devices using first-principles calculations in combination with the Boltzmann transport theory and non-equilibrium/equilibrium molecular dynamics (NEMD/EMD).

- **Impurities Behavior in Iron:** Multi-scale simulation of foreign impurities behavior in iron (carbon/defects interaction, carbon diffusion and clustering, phase transformation, hydrogen/defects interaction, hydrogen segregation at grain boundary, etc.) using first-principles methods in combination with classical molecular dynamics (MD), kinetic Monte Carlo (kMC), cluster expansion and variation methods (CEM/CVM) for designing highly-tuned strength, ductility and fracture toughness steel as well as improving the production process of steel. Development of new Tersoff/ZBL interatomic potential for Fe-C, Fe-N binary systems and new embedded-atom method (EAM) interatomic potential for Fe-C-H ternary system using evolutionary algorithm and machine learning (artificial neural networks).

- **Diesel Oxidation Catalysts:** First-principles based simulation of the reactivity toward the adsorption/dissociation and oxidation/reduction of molecules (O_2, NO, C_xH_y, etc.) on metal oxide supported metal cluster as well as metallic bilayer materials for designing advanced diesel oxidation catalysts and cathode catalysts of fuel cells.

- **Molecular Devices:** First-principles based simulation of the electronic and magnetic properties of metallo-macrocycles (phthalocyanine and porphyrin based structures) as well as their interaction with diatomic molecules for designing sensitive and selective molecular electronic devices (for gas sensor application).

✶ *Except for the first-principles calculations (VASP), molecular dynamics (LAMMPS) and artificial neural networks codes (ÆNET), all the computational codes used or being used are self-developed.*

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:** Institute of Physics (IOP), United Kingdom Select Paper: "*Another way of looking at bonding on bimetallic surfaces: The role of spin polarization of surface metal d-states*"
- **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

FELLOWSHIPS/SCHOLARSHIPS

- **2015/12 - 2020/03:** Building of Consortia for the Development of Human Resources in Science and Technology project, implemented by the Ministry of Education, Culture, Sports, Science and Technology (MEXT) of Japan
- **2008/10 - 2013/09:** Japanese Ministry of Education, Culture, Sports, Science and Technology (MEXT) Scholarship under Quantum Engineering Design Program
- **2007/01 - 2007/12:** Japan Student Services Organization (JASSO) Scholarship under Student Exchange Support Program

RESEARCH FUNDS ACQUISITION

External (As a Principal Investigator):

Research topic: "*Atomistic materials design of new heterogeneous iron/steel*"
Project Period: 2015/12 - 2020/03
Research Institution: Osaka University
Supported by: PCoMS (Professional development Consortium for Computational Materials Scientists under the Building of Consortia for the Development of Human Resources in Science and Technology project, implemented by the Ministry of Education, Culture, Sports, Science and Technology of Japan (MEXT) and the Japan Science and Technology Agency (JST))

External (As a Contributor):

Research topic: "*Investigation into unusual behaviors in electron and lattice thermal conductivity*"
Grant Number: JP-MJCR18I2
Project Period: 2018/04 - 2023/03
Research Institution: Osaka University
Supported by: The Core Research for Evolutional Science and Technology (CREST) of the Japan Science and Technology Agency (JST)

Internal Competitive Funds:

- **Research topic:** "*A theoretical study of dynamics and characteristics of oxygen reduction reaction for new catalyst development*"
  Project Period: 2012/04 - 2013/03
  Research Institution: Osaka University
  Supported by: Japan GCOE (Global Center of Excellence) Program "Center of Excellence for Atomically Controlled Fabrication Technology"
  Research Team: Ferensa Oemry, Tien Quang Nguyen, Saputro Adhitya Gandaryus, Koji Shimizu and Chong Kong Ng
- **Research topic:** "*Theoretical analysis on the application to electronic devices using organic materials*"
  Project Period: 2011/04 - 2012/03
  Research Institution: Osaka University
  Supported by: Japan GCOE (Global Center of Excellence) Program "Center of Excellence for Atomically Controlled Fabrication Technology"
  Research Team: Tien Quang Nguyen, Aspera Susan Meñez, Wungu Triati Dewi Kencana, Moreno Joaquin Lorenzo Valmoria, Saputro Adhitya Gandaryus and Yohei Ushijima
- **Research topic:** "*Design of thin film nano-devices using simulation technology*"
  Project Period: 2009/04 - 2010/03
  Research Institution: Osaka University

Supported by: Japan GCOE (Global Center of Excellence) Program "Center of Excellence for Atomically Controlled Fabrication Technology"
Research Team: Tien Quang Nguyen, Hirofumi Kishi, Mary Clare Sison Escaño, Abdulla Ali Abdulla Sarhan and Ferensa Oemry

INDUSTRIAL COLLABORATION

- **Nippon Steel** (**PCoMS** Project): Carbon Diffusion and Clustering in Iron (2016-2020)
- **JFE Steel (ISMA** Project): Hydrogen Behavior in Iron/Steel (2013-2015)
- **TANAKA Precious Metals Group** Project: Cathode Catalysts for Fuel Cells (2013)
- **ISUZU Motors Inc.** Project: Diesel Oxidation Catalyst for Car Exhaust Filters (2008-2013)
- **SHARP Corporation** Project: Molecular Electronic Devices for Gas Sensors (2007-2009)

RESEARCH VISITS

Location: Institute for Materials Science, Tohoku University
Host: Prof. Tetsuo Mohri
Periods of stays: ●2020/01/14-28 (2 weeks) ●2019/09/30-10/11 (2 weeks) ●2018/12/03-14 (2 weeks) ●2018/06/04-15 (2 weeks) ●2017/07/24-08/04 (2 weeks) ●2017/01/16-30 (2 weeks)
Research topic: Cluster expansion/variation methods and their applications for studying multi-component alloys (iron-carbon alloy, high-entropy alloys)

COMPUTER SKILLS AND OUTPUTS

Skills:
- Operating systems: Windows, macOS, Linux (Fedora, Ubuntu, SuSE, CentOS)
- Programing languages: Very experienced in FORTRAN, MATLAB; knowledgable in C/C++, Python, MPI, Shell-scripts, Mathematica, HTML, Markdown, LaTeX
- Simulation packages: VASP, STATE-Senri, AkaiKKR, LAMMPS, Phonopy, Wannier90, BoltzWann, BoltzTraP
- Visualization softwares: GNUplot, Matplotlib, VESTA, CrystalMaker, Ovito

Self-developed Programs:
- Fortran program for calculation of the chemical potential and Seebeck coefficient of impurity-doped semiconductor systems
- 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 high entropy alloys 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 for fuel cell catalysts
- Fortran utilities for analysis/manipulating output data of VASP and LAMMPS
- Python program for calculation of interface resistance in bimetallic systems (spintronics)
- MATLAB Graphic User Interface program for Visualizing Hydrogen Atomic Orbitals

Computing Facility Management
- **2015/12 - present**: Built own high-performance computing cluster and have been maintaining it
- **2008/10 - 2013/09**: Supported the management of research group's computing facility
- **2009/12 - 2017/11**: Set up computational facilities and in charge for the practical hands-on section for the Asia Computational Materials Design (CMD®) Workshops overseas (in Vietnam, Thailand and Philippines)

EDUCATION ACHIEVEMENTS

Dissertation Supervision:
- **2017/09 - 2019/08:**
  Number of students: 1 Status: Completed
  Academic degree: Master of Engineering
  Institution: Vietnam-Japan University (VJU-VNU)
  Thesis title: "*Atomistically kinematic simulations of carbon diffusion in α-iron with point defects*"
- **2016/09 - 2018/08:**
  Number of students: 1 Status: Completed
  Academic degree: Master of Engineering
  Institution: Vietnam-Japan University (VJU-VNU)
  Thesis title: "*Computational kinetics on diffusion process of carbon in iron bulk*"

Dissertation Co-supervision or Guidance:

- **2020/04 - present:**
  Number of students: 1 Status: On going
  Academic degree to be acquired: Doctor of Philosophy in Engineering
  Institution: Osaka University
  Research topics: "*Thermoelectric materials*"
- **2018/10 - present:**
  Number of students: 1 Status: On going
  Academic degree to be acquired: Doctor of Philosophy in Engineering
  Institution: Osaka University
  Research topics: "*Impurities behavior in iron/steel*"
- **2013/10 - 2015/09:**
  Number of students: 1 Status: Completed
  Academic degree: Doctor of Philosophy in Engineering
  Institution: Osaka University
  Thesis title: "*Theoretical study on the role of oxygen vacancy in the improvement of metal oxides' reactivity for green technology applications*"

Construction of Teaching Resource:

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 final exams.
Teaching Level: Graduate students

Invited Public Lectures:

- "*Interatomic potentials development of Fe-C binary system for atomistic materials design of new heterogenous iron*"
  Lecture for students at Faculty of Physics, Hanoi National University of Education
  2016/11/04, Hanoi, Vietnam
- "*Computational Materials Design for energy and environmental applications*"
  Lecture for students at Faculty of Physics, VNU University of Science, Vietnam National University (Hanoi)
  2012/12/06-08, Hanoi, Vietnam

Practice Guidance at Scientific Workshops/Schools:

- The 9th Asia CMD® Workshop (2017/11/29-12/01, Vietnam-Japan University, Hanoi, Vietnam)
- The 5th Asia CMD® Workshop (2013/12/05-07, VNU University of Science, VNUH, Hanoi, Vietnam)
- The 4th Asia CMD® Workshop (2012/12/06-08, VNU University of Science, VNUH, Hanoi, Vietnam)
- The 3rd Asia CMD® Workshop (2011/12/09-11, Saigon University, Ho Chi Minh City, Vietnam)
- The 1st Asia CMD® Workshop (2011/02/15-17, Mahidol University, Bangkok, Thailand)
- The 2nd Asia CMD® Workshop (2010/12/16-18, Hue University, Hue, Vietnam)
- The 1st Asia CMD® Workshop (2009/12/16-18, VNU University of Science, VNUH, Hanoi, Vietnam)

Other Activities:

- Collaborative teaching at Vietnam-Japan University (on-site and remote lectures)
- Designed, constructed (in HTML/CSS programming languages) and maintained the official website of the Quantum Engineering Design Course (English Graduate Course Program of the Graduate School of Engineering, Osaka University: http://www.dyn.ap.eng.osaka-u.ac.jp/QEDC) during my graduate studies.
- Co-designed and advised on the construction of the official website of the Master's Program in Nanotechnology (English Graduate Course of Vietnam-Japan University, Vietnam National University (Hanoi): http://mnt.vju.ac.vn/).

RESEARCH ACHIEVEMENTS

Patents (Registered):

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 and English (Translated)
Patent Number: JP2011080798-A
Published Date: Apr 21, 2011
Inventors (in Alphabetical Order): Keita Hara, Hideaki Kasai, Tsunehisa Kawada, Hiroshi Nakanishi, Mieko Otonashi, Tien Quang Nguyen, Mikihiro Yamanaka
International Patent Classification: G01N-027/12 (or G01N 27/12)

Review Articles and Books:

1. Mary Clare Sison Escaño, 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 Escaño 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. Ngoc Nam Ho, Ryo Yamada, Haruki Okumura, Tien Quang Nguyen, Katsuhiro Suzuki, Hikari Shinya, Akira Masago, Tetsuya Fukushima and Kazunori Sato
"*Intrinsic defect formation and effect of transition-metals doping on transport property in ductile thermoelectric material α-Ag_2S: First-principles study*"
Physical Chemistry Chemical Physics (2021)
2. 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*"
Solid State Communications **323** (2021) 114115(1-5) - https://arxiv.org/abs/2001.10191
3. Mary Clare Sison Escaño and Tien Quang Nguyen
"*Does GaAs bulk lattice really expand due to defects in the low concentration regime?*"
Solid State Communications **316** (2020) 113918(1-6)
4. Mary Clare Sison Escaño, 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(1-7)
5. Tien Quang Nguyen, Mary Clare Sison Escaño, 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
6. Mary Clare Sison Escaño, 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)
7. 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
8. 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
9. Mary Clare Sison Escaño, 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
10. Mary Clare Sison Escaño, 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
11. 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
12. Tien Quang Nguyen, Mary Clare Sison Escaño, 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
13. Tien Quang Nguyen, Allan Abraham Bustria Padama, Mary Clare Sison Escaño 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
14. Mary Clare Sison Escaño, Tien Quang Nguyen and Hideaki Kasai
"*Molecular oxygen adsorption on ferromagnetic platinum*"
Chemical Physics Letters, **555** (2013) 125-130
15. 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
16. Mary Clare Sison Escaño, 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

17. Mary Clare Sison Escaño, 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)
18. Tien Quang Nguyen, Mary Clare Sison Escaño and Hideaki Kasai
"*Nitric oxide adsorption effects on metal phthalocyanines*"
Journal of Physical Chemistry B, **114** (2010) 10017-10021
19. Mary Clare Sison Escaño, 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)
20. Tien Quang Nguyen, Susan Meñez Aspera, Hiroshi Nakanishi and Hideaki Kasai
"*NO adsorption effects on various functional molecular nanowires*"
Computational Materials Science, **47** (2009) 111-120
21. Tien Quang Nguyen, Mary Clare Sison Escaño, 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)
22. Mary Clare Sison Escaño, 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
23. Tien Quang Nguyen, Mary Clare Sison Escaño, 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)
24. Tien Quang Nguyen, Mary Clare Sison Escaño, 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
25. 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, Yayoi Terada and Tetsuo Mohri
"*Entropy of a High-Entropy Alloy*"
IMR KINKEN Research Highlights 2020
Online ISSN: 1883-0315
2. Tien Quang Nguyen, Ngoc Nam Ho, Kazunori Sato and Yoji Shibutani
"*Atomistically kinetic simulations of carbon diffusion in α-Fe with point defect*"
Proceedings of the Computational Mechanics Conference, Volume **2019.32** (2019) 250(1-4)
Online ISSN: 2424-2799
3. 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
(2019/05/06, Vietnam-Japan University)
4. 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 **2018.31** (2018) 237(1-4)
Online ISSN: 2424-2799
5. Mary Clare Sison Escaño, 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. Thi Dung Pham, Tien Quang Nguyen, Tomoyuki Terai, Yoji Shibutani, Masaaki Sugiyama and Kazunori Sato
"*First-principles study on segregation of carbon in α-Fe <110> symmetrical tilt grain boundaries*"
Materials Transactions (2021)
2. Tien Quang Nguyen, Ngoc Nam Ho, Katsuhiro Suzuki, Hikari Shinya, Akira Masago, Tetsuya Fukushima, Kazunori Sato
"*Enhancement of Seebeck coefficient of SiGe alloy by transition metal doping: A first-principles investigation*"
Journal of Chemical Physics (2021)
3. Maria Herminia Balgos, Mary Clare Sison Escaño, Rafael Jaculbia, Tien Quang Nguyen, Elizabeth Ann Prieto, Elmer Estacio, Arnel Salvador, Armando Somintac, Masahiko Tani, Norihiko Hayazawa and Yousoo Kim
"*Revisiting the structure and electronic property of the arsenic antisite defect in gallium arsenide*"
Applied Surface Science (2021)

4. Tien Quang Nguyen, Kazunori Sato and Yoji Shibutani
"*Kinetic Monte Carlo study on the diffusion properties and clustering of carbon in Fe-C alloy*"
Modelling and Simulation in Materials Science and Engineering (2021)
5. Tien Quang Nguyen, Kazunori Sato and Yoji Shibutani
"*Effects of low carbon content on the tetragonality of iron lattice*"
Materials Transactions (2021)

Invited Talks:
1. "*Kinetic Monte Carlo simulations of carbon diffusion in bcc iron with point defects*"
Invited talk at the Institute for Materials Research, Tohoku University
2019/10/08, Miyagi, Japan
2. "*Atomistically kinetic simulations of carbon behavior in bcc iron with point defect*"
Invited talk at the Short-talk Session of the 35th Computational Materials Design, Osaka University
2019/09/02-06, Osaka, Japan
3. "*Diffusion properties of carbon and tetragonality effect in Fe-C alloy*"
Invited talk at the Institute for Materials Research, Tohoku University
2018/12/06, Miyagi, Japan
4. "*Computational kinetics on diffusion of carbons in bcc iron*"
Invited talk at the Institute for Materials Research, Tohoku University
2018/06/07, Miyagi, Japan
5. "*Analytic interatomic potential for modeling phase transformation in the Fe-C system*"
Invited talk at the Institute for Materials Research, Tohoku University
2017/08/02, Miyagi, Japan
6. "*Analytic bond-order potential for atomistic simulations of Fe-C system*"
Invited talk at the Center for Computational Materials Science, Institute for Materials Research, Tohoku University
2017/01/18, Miyagi, Japan
7. "*Development of interatomic potentials for modeling of hydrogen and carbon interaction near lattice defects in bcc iron*"
Invited talk at the Center for Atomic and Molecular Technologies, Graduate School of Engineering, Osaka University
2016/04/28, Osaka, Japan
8. "*First-principles study on NO adsorption and oxidation on metallo-macrocycles and ceria-supported Pt cluster*"
Invited talk at the Mini Symposium on Computational Chemistry for Material Applications, The National University of Malaysia
2013/07/15-16, Selangor, Malaysia
9. "*Porphyrins and macrocycles: From basics to applications*"
Invited talk at the ECS 221st Meeting
2012/05/06-10, Washington State Convention Center, Seattle, Washington, USA

Scientific Seminars:
1. "*First-principles calculations of Seebeck coefficient in 3d-transition metal doped SiGe alloys*"
Research Colloquium at Sato Laboratory, Graduate School of Engineering, Osaka University
2020/11/05, Osaka, Japan
2. "*Atomistically kinetic simulation of carbon clustering in bcc iron*"
Research Colloquium at Sato Laboratory, Graduate School of Engineering, Osaka University
2020/07/02, Osaka, 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, Osaka University
2018/05/15, 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, Graduate School of Engineering, Osaka University
2017/10/06, Osaka, Japan
5. "*Analytic bond-order potential for atomistic simulations of Fe-C system*"
Scientific Seminar at Kakeshita Laboratory, Graduate School of Engineering, Osaka University
2017/04/14, Osaka, Japan
6. "*Hydrogen behaviors in steels: Hydrogen/carbon/vacancy interaction*"
Scientific Seminar at Ogata Laboratory, Graduate School of Engineering Science, Osaka University
2015/06/17, Osaka, Japan
7. "*Uranium: The metal of tomorrow*"
Nandemo Seminar at Kasai Laboratory, Graduate School of Engineering, Osaka University
2013/11/15, Osaka, Japan
8. "*NO oxidation on CeO_2-supported Pt_4 cluster*"
Project Seminar at ISUZU Advanced Engineering Center, Isuzu Motors Fujisawa Plant
2013/02/08, Kanagawa, Japan

9. "*Nitric oxide adsorption on oxygen pre-covered Pt_4/CeO_2*"
   Project Seminar at ISUZU Advanced Engineering Center, Isuzu Motors Fujisawa Plant
   2011/07/13, Kanagawa, Japan

Oral Presentations in International Conferences:

1. "*Enhancement of Seebeck coefficient of SiGe alloy by transition metal doping: A first-principles investigation*"
   The 168th Annual Spring Meeting of the Japan Institute of Metals and Materials‡
   2021/03/16-19, Online via Zoom
2. "*Carbon clustering in bcc iron: A kinetic Monte Carlo study*"
   PCoMS Symposium & Annual Meeting of Supercomputing Consortium for Computational Materials Science 2020‡
   2021/02/15-16, Online via Zoom
3. "*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†
   2020/03/17-19, Tokyo Institute of Technology, Tokyo, Japan
4. "*Atomistic kinematics of carbon diffusion and clustering in bcc Fe with point defects*"
   APS March Meeting 2020†
   2020/03/02-06, Colorado Convention Center, Denver, Colorado, USA
5. "*Carbon diffusion and clustering in bcc iron: A kinetic Monte Carlo study*"
   Workshop on Nanotechnology-Driven Topics
   2019/12/10, Osaka University, Osaka, Japan
6. "*Atomistic simulations of carbon behavior in bcc iron with point defect*"
   PCoMS Symposium & Annual Meeting of Supercomputing Consortium for Computational Materials Science 2019
   2019/10/24-25, Tohoku University, Miyagi, Japan
7. "*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
   2019/09/16-18, Toyo University, Saitama, Japan
8. "*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
   2019/03/20-22, Tokyo Denki University, Tokyo, Japan
9. "*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
   2018/11/23-25, Tokushima University, Tokushima, Japan
10. "*Diffusion properties of carbon in a-Fe*"
    PCoMS Symposium & Annual Meeting of Supercomputing Consortium for Computational Materials Science 2018
    2018/10/22-23, Tohoku University, Miyagi, Japan
11. "*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
    2018/09/19-21, Tohoku University, Miyagi, Japan
12. "*Construction of interatomic potential for Fe-C systems using evolutionary algorithm*"
    APS March Meeting 2018
    2018/03/05-09, Los Angeles Convention Center, Los Angeles, California, USA
13. "*Interatomic potentials for carbon in iron based on density functional theory*"
    PCoMS Symposium & Annual Meeting of Supercomputing Consortium for Computational Materials Science 2017
    2017/11/09-10, Tohoku University, Miyagi, Japan
14. "*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
    2017/09/06-08, Hokkaido University, Hokkaido, Japan
15. "*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
    2016/10/17-18, Tohoku University, Miyagi, Japan
16. "*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
    2016/03/24-26, Osaka University, Osaka, Japan
17. "*Atomistic materials design of new iron with highly-tuned strength, ductility and fracture toughness: Interatomic potential development*"
    PCoMS Kick-off Meeting
    2016/02/26, Tohoku University, Tokyo, Japan
18. "*NO oxidation on CeO_2-supported Pt_4 cluster: A DFT+U study*"
    Quantum Engineering Design Workshop

2013/10/25, Osaka University, Osaka, Japan
19. "*NO oxidation on O pre-covered Pt_4/CeO_2*"
OU-TUM Workshop: Trends in Catalysis
2013/05/16, Osaka University, Osaka, Japan
20. "*Theoretical Investigation on NO oxidation on O pre-covered Pt_4/CeO_2*"
International Workshop on the Theory of Dense Kondo Systems
2013/03/19-20, Osaka University, Osaka, Japan
21. "*DFT+U investigation on the adsorption and dissociation of oxygen on Pt-coated Ceria*"
International Workshop on Current Surface Science Trend
2012/11/08, Osaka University, Osaka, Japan
22. "*Oxidation of metal and metal oxide systems*"
Asia Computational Materials Design Workshop
2011/10/10-12, De La Salle University, Manila, Philippines
23. "*Computational Materials Design case studies: Oxidation of metal/metal oxide systems*"
International Conference on Quantum Simulations and Design
2011/09/27-29, Max Planck Institute, Dresden, Germany
24. "*First-principles study on nitric oxide adsorption on metal tape-porphyrines*"
Asia Computational Materials Design Workshop
2011/02/15-17, Mahidol University, Bangkok, Thailand
25. "*Adsorption of nitric oxide on metal porphyrin tape*"
Asia Computational Materials Design Workshop
2010/12/16-18, Hue University, Hue, Vietnam
26. "*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
2010/05/30-06/04, Osaka University, Osaka, Japan
27. "*Nitric oxide adsorption effects on metal phthalocyanines*"
OU-DLSU Academic Research Workshop
2010/05/27-28, Osaka University, Osaka, Japan
28. "*The role of metal porphyrin tape as sensor in detecting NO gas*"
Asia Computational Materials Design Workshop
2009/11/26-28, Ha-Noi University of Science, Ha-Noi, Vietnam
29. "*NO adsorption effects on metal tape-porphyrins*"
GCOE International Workshop
2008/11/25-27, Osaka University, Osaka, Japan
30. "*The adsorption of NO on various metal tape-porphyrins*"
ITB-OU Academic Research Workshop
2008/06/30, Osaka University, Osaka, Japan
31. "*DFT study on the binding of CO, NO, and O_2 to iron tape-porphyrin*"
International Workshop on Quantum Simulation 2007
2007/09/13, Osaka University, Osaka, Japan
32. "*O_2 adsorption effects on electronic properties of Fe tape-porphyrin*"
International Science and Engineering Workshop
2007/05/15, Osaka University, Osaka, Japan
33. "*DFT study on O_2 adsorbed Fe tape-porphyrin*"
The 3rd International Workshop on Reactions Involving Oxygen
2007/05/10, Osaka University, Osaka, Japan
34. "*Study of electronic properties of perovskite $BaTiO_3$*"
The 4th Workshop on Simulation & Modeling Physics
2006/11/22-24, 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)
2019/10/28-30, Osaka University, Osaka, Japan
2. "*Hydrogen and carbon interactions near lattice defects in bcc iron by combined theoretical methods*"
2015 MRS Fall Meeting & Exhibit
2015/11/29-12/04, Boston, Massachusetts, USA
3. "*Atomistic modeling of hydrogen-vacancy-carbon interaction in α-iron*"
The 9th International Conference on Computational Physics
2015/01/07-11, 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
2014/12/20-22, 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
2013/11/26-28, 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
2012/11/14-16, 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
2012/10/22-24, Osaka University, Osaka, Japan
8. "*Spin effects in metal surface reactions: O_2 on ferromagnetic Pt*"
AVS 58th International Symposium & Exhibition
2011/10/30-11/04, Nashville Convention Center, Nashville, Tennessee, USA
9. "*Oxygen dissociation on metal oxide-supported Pt cluster*"
The 4th International Symposium on Atomically Controlled Fabrication Technology
2011/10/31-11/02, Osaka University, Osaka, Japan
10. "*Oxygen dissociative adsorption on $Pt_4/CeO_2(111)$ surface*"
The First JSMS Symposium on Multiscale Materials Modeling
2011/05/23-24, 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
2010/11/24-26, 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
2010/08/29-09/03, 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
2010/05/30-06/04, 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
2009/11/08-13, 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
2009/09/25-28, Kumamoto University, Kumamoto, Japan
16. "*Theoretical study on interaction of NO with metal tape-porphyrins*"
First International Symposium on Atomically Controlled Fabrication Technology
2009/02/16-17, Osaka University, Osaka, Japan
17. "*DFT study on the adsorption of NO on various metal tape-porphyrins*"
International Symposium on Surface Science and Nanotechnology
2008/11/09-13, 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
2008/05/31-06/03, 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
2007/10/15-17, 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
2007/09/26-28, Osaka University, Osaka, Japan
21. "*DFT study of Jahn-Teller effect in $BaTiO_3$*"
The 3rd International Workshop on Nanophysics and Nanotechnology
2006/12/06-09, Ha-Long, Vietnam
22. "*Calculation of electronic properties of $BaTiO_3$ using DFT method*"
HUS Scientific Conference
2006/11/11, Ha-Noi University of Science, Ha-Noi, Vietnam
23. "*First-principles calculation for $BaTiO_3$*"
The 31st National Conference on Theoretical Physics
2006/08/22-25, Hon-Ngu Hotel, Cua-Lo, Nghe-An, Vietnam

SOCIAL ACTIVITIES

Organized Workshops (Overseas):

- The 9th Asia Computational Materials Design (CMD®) Workshop
2017/11/29-12/01, Vietnam-Japan University, Hanoi, Vietnam
- The 5th Asia Computational Materials Design (CMD®) Workshop
2013/12/05-07, VNU University of Science, VNUH, Hanoi, Vietnam

- The 4th Asia Computational Materials Design (CMD®) Workshop
  2012/12/06-08, VNU University of Science, VNUH, Hanoi, Vietnam
- The 3rd Asia Computational Materials Design (CMD®) Workshop
  2011/12/09-11, Saigon University, Ho Chi Minh City, Vietnam
- The 1st Asia Computational Materials Design (CMD®) Workshop
  2011/02/15-17, Mahidol University, Bangkok, Thailand
- The 2nd Asia Computational Materials Design (CMD®) Workshop
  2010/12/16-18, Hue University, Hue, Vietnam
- The 1st Asia Computational Materials Design (CMD®) Workshop
  2009/12/16-18, VNU University of Science, VNUH, Hanoi, Vietnam

Organized Workshops (Japan):
- HUS-OU-UBC International Workshop on Quantum Design and Realization
  2012/02/27-28, Osaka University, Osaka, Japan
- HUS-OU-BBK Scientific Workshop
  2010/11/22, Osaka University, Osaka, Japan
- HUS-OU International Workshop on Quantum Simulation
  2008/09/12, Osaka University, Osaka, Japan
- HUS-OU International Workshop on Quantum Simulation
  2007/09/13, Osaka University, Osaka, Japan

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 (since 2017)
- American Physical Society (since 2018)
- Materials Research Society (since 2015, inactive)
- American Vacuum Society (since 2009, inactive)
- The Physical Society of Japan (since 2009, inactive)
- Vietnam Theoretical Physics Society (since 2006)

LIST OF REFERENCES

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  ResearchMap URL: https://researchmap.jp/read0076412

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†No presentation due to COVID-19 pandemic
‡Online presentation due to COVID-19 pandemic

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