

## CURRICULUM VITAE

### NGUYEN TIEN QUANG

#### Current Affiliation:

Shinshu University  
Research Initiative for Supra-Materials (RISM)  
Data-Driven AI Laboratory  
4-17-1 Wakasato, Nagano-shi, Nagano 380-8553, JAPAN

#### Contact Information:

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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
  - **Date of Birth:** Oct 06, 1982
  - **Language Proficiency:** Vietnamese (native), English (fluent), Japanese (basic)
- Nationality:** Vietnamese  
**Place of Birth:** Binh-Phuoc, Vietnam

## 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 and Mathematical 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

- **2022/04 - present: Shinshu University (Research Initiative for Supra-Materials)**  
**Position:** Specially-Appointed Assistant Professor (full-time)  
**Main Duties:** Doing research on Solid-Liquid Interfaces and High-Entropy Ceramics
- **2020/04 - 2022/03: 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 - 2022/03: Osaka University (Graduate School of Engineering)**  
**Duties:** Co-supervising doctor course students' theses
- **2017/05 - 2022/03: 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<sub>2</sub>, NO, C<sub>x</sub>H<sub>y</sub>, 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 (ENET), 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<sub>2</sub> on ferromagnetic Pt/M*” at the 54<sup>th</sup> Annual Symposium of the Vacuum Society of Japan
- **2011:** Best Poster Award for the presentation entitled “*Study of NO oxidation reaction over Pt cluster supported on  $\gamma$ -Al<sub>2</sub>O<sub>3</sub>(111) surface*” at the 4<sup>th</sup> International Symposium on Atomically Controlled Fabrication Technology
- **2009:** Institute of Physics (IOP), United Kingdom Selected 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 Contributor):

**Research Topic:** “*Investigation into unusual behaviors in electron and lattice thermal conductivity*”

**Grant Number:** JP-MJCR18I2

**Project Period:** 2018/10 - 2024/03

**Research Institution:** Osaka University

**Total Amount:** 150-500 million yen (for 5 institutions)

**Supported By:** The Core Research for Evolutional Science and Technology (CREST) of the Japan Science and Technology Agency (JST)

### 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

**Total Amount:** 14,420,000 yen

**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))

### 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

- **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)
- Programming languages: Very experienced in FORTRAN, MATLAB; knowledgeable 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 module for integrating into AkaiKKR program to calculate thermoelectric properties (Seebeck coefficient, electrical conductivity, electron thermal conductivity) in disordered alloys
- Fortran program for calculating atomic mean-squared displacements from phonon density of states
- Fortran program for calculating of chemical potential and Seebeck coefficient of impurity-doped semiconductor systems from electron density of states
- 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 finding Tersoff potentials for binary/ternary system using Genetic Algorithm
- Fortran program for finding 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/Python utilities for analysing/manipulating output data of VASP, LAMMPS, AkaiKKR, and BoltzWann
- Python program for calculating of interface resistance in bimetallic systems (spintronics)
- MATLAB Graphic User Interface program for Visualizing Hydrogen Atomic Orbitals

### Computing Facility Management

- **2015/12 - 2022/03:** 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  
Academic degree: Master of Engineering
- Status: Completed

Institution: Vietnam-Japan University (VJU-VNU)

Thesis title: “Atomistically kinematic simulations of carbon diffusion in  $\alpha$ -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 - 2022/10:**

Number of students: 1

Status: Completed

Academic degree to be acquired: Doctor of Philosophy in Engineering

Institution: Osaka University

Research topics: “Thermoelectric materials”

- **2018/10 - 2022/03:**

Number of students: 1

Status: Completed

Academic degree to be acquired: Doctor of Philosophy in Engineering

Institution: Osaka University

Research topics: “Interaction between carbon and extended defects in Fe studied by the first-principles based interatomic potential”

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

**Type:** Granted, International

**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  
Edited by M. Aliofkhazraei, N. Ali, W. I. Milne, C. S. Ozkan, S. Mitura, and J. L. Gervasoni  
Taylor & Francis Group, New York, 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  
Edited by A. Kaibara and G. Matsumura  
Nova Science Publishers, New York, USA (2012) 229-260  
ISBN: 9781620810682

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

1. Ngoc Nam Ho, Katsuhiro Suzuki, Akira Masago, [Tien Quang Nguyen](#), Hikari Shinya, Tetsuya Fukushima and Kazunori Sato  
“Ascertaining electrical conductivity of  $\text{Ag}_2\text{S}_{1-x}\text{Se}_x$  ( $x = 0, 0.25, 0.50$ ): Electron-phonon coupling investigation”  
Applied Physics Letters (2022) | Status: Accepted
2. 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  
“Atomically precise delineation of As antisite defect states from undoped gallium arsenide host lattice by STM/STS measurements and DFT calculations”  
Physica Status Solidi B (2022) | Status: Accepted
3. Thi Dung Pham, [Tien Quang Nguyen](#), Tomoyuki Terai, Yoji Shibutani, Masaaki Sugiyama and Kazunori Sato  
“Interaction between carbon and extended defects in  $\alpha$ -iron studied by first-principles based interatomic potential”  
Materials Transactions **63** (2022) 475-483
4. Ngoc Nam Ho, Katsuhiro Suzuki, [Tien Quang Nguyen](#), Hikari Shinya, Akira Masago, Tetsuya Fukushima and Kazunori Sato  
“Low-temperature acanthite-like phase of  $\text{Cu}_2\text{S}$ : electronic and transport properties”  
Physical Review B **105** (2022) 075205(1-11)
5. Tsukasa Terada, Yuto Uematsu, Takafumi Ishibe, Nobuyasu Naruse, Kazunori Sato, [Tien Quang Nguyen](#), Eiichi Kobayashi, Yuichiro Yamashita, Hideyuki Nakano and Yoshiaki Nakamura  
“Giant enhancement of Seebeck coefficient by deformation of silicene buckled structure in calcium-intercalated layered silicene film”  
Advanced Materials Interfaces **9** (2022) 2101752(1-7)
6. Tsukasa Terada, Takafumi Ishibe, Toranosuke Katayama, Kazunori Sato, [Tien Quang Nguyen](#), Hideyuki Nakano and Yoshiaki Nakamura  
“Thermoelectric power factor enhancement of calcium-intercalated layered silicene by introducing metastable phase”  
Applied Physics Express **14** (2021) 115505(1-4)
7. Thi Dung Pham, [Tien Quang Nguyen](#), Tomoyuki Terai, Yoji Shibutani, Masaaki Sugiyama and Kazunori Sato  
“Segregation of carbon in  $\alpha$ -Fe symmetrical tilt grain boundaries studied by first-principles based interatomic potential”  
Materials Transactions **62** (2021) 1057-1063
8. Ngoc Nam Ho, Ryo Yamada, Haruki Okumura, [Tien Quang Nguyen](#), Katsuhiro Suzuki, Hikari Shinya, Akira Masago, Tetsuya Fukushima and Kazunori Sato  
“Correction: Intrinsic defect formation and effect of transition-metals doping on transport property in ductile thermoelectric material  $\alpha$ - $\text{Ag}_2\text{S}$ : First-principles study”  
Physical Chemistry Chemical Physics **23** (2021) 8938
9. 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  $\alpha$ - $\text{Ag}_2\text{S}$ : First-principles study”

- Physical Chemistry Chemical Physics **23** (2021) 9773-9784
10. 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>
  11. 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)
  12. 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)
  13. 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
  14. 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)
  15. Tien Quang Nguyen, Kazunori Sato and Yoji Shibutani  
*"Development of Fe-C interatomic potential for carbon impurities in  $\alpha$ -iron"*  
Computational Materials Science **150** (2018) 510-516
  16. 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
  17. 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
  18. 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
  19. Nguyen Hoang Linh, Tien Quang Nguyen, Wilson Agerico Dino and Hideaki Kasai  
*"Effect of oxygen vacancy on the adsorption of O<sub>2</sub> on anatase TiO<sub>2</sub>(001): A DFT-based study"*  
Surface Science, **633** (2015) 38-45
  20. 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<sub>2</sub>-supported platinum cluster"*  
Applied Surface Science, **288** (2014) 244-250
  21. 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
  22. Mary Clare Sison Escaño, Tien Quang Nguyen and Hideaki Kasai  
*"Molecular oxygen adsorption on ferromagnetic platinum"*  
Chemical Physics Letters, **555** (2013) 125-130
  23. Hirofumi Kishi, Ferensa Oemry, Tien Quang Nguyen, Shinichi Kunikata, Hiroshi Nakanishi, Hideaki Kasai, Hiroyoshi Maekawa and Kazuo Osumi  
*"Study of NO oxidation reaction over the Pt cluster supported on  $\gamma$ -Al<sub>2</sub>O<sub>3</sub>(111) surface"*  
Current Applied Physics, **12** (2012) S110-S114
  24. 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
  25. 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)
  26. 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
  27. 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)
  28. 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
  29. 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)
30. 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
  31. 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)
  32. 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
  33. Tien Quang Nguyen and Thanh Cong Bach  
“First-principles calculation for BaTiO<sub>3</sub>”  
Communications in Physics, **17** (2007) 128-133

#### Other Articles (Proceedings, Highlights,...):

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  $\alpha$ -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, Volume **2019**, 114(1-2)  
(2019/05/04, 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. Tien Quang Nguyen, Ngoc Nam Ho, Katsuhiko Suzuki, Hikari Shinya, Akira Masago, Tetsuya Fukushima and Kazunori Sato  
“Enhancement of Seebeck coefficient of SiGe alloy by transition metal doping: A first-principles investigation”  
Journal of Chemical Physics (2022)
2. 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 (2022)
3. Tien Quang Nguyen, Kazunori Sato and Yoji Shibutani  
“Effects of low carbon content on the tetragonality of iron lattice”  
Materials Transactions (2022)

#### 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 35<sup>th</sup> 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. “*Thermoelectric properties of random alloys*”  
Research Colloquium at Sato Laboratory, Graduate School of Engineering, Osaka University  
2021/11/04, Osaka, Japan
2. “*First-principles calculations of thermal transport properties in transition metal doped SiGe alloys*”  
Research Colloquium at Sato Laboratory, Graduate School of Engineering, Osaka University  
2021/06/10, Osaka, Japan
3. “*An introduction to thermoelectricity*”  
Research Colloquium at Sato Laboratory, Graduate School of Engineering, Osaka University  
2021/05/06, Osaka, Japan
4. “*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
5. “*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
6. “*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
7. “*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
8. “*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
9. “*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
10. “*Uranium: The metal of tomorrow*”  
Nandemo Seminar at Kasai Laboratory, Graduate School of Engineering, Osaka University  
2013/11/15, Osaka, Japan
11. “*NO oxidation on CeO<sub>2</sub>-supported Pt<sub>4</sub> cluster*”  
Project Seminar at ISUZU Advanced Engineering Center, Isuzu Motors Fujisawa Plant  
2013/02/08, Kanagawa, Japan
12. “*Nitric oxide adsorption on oxygen pre-covered Pt<sub>4</sub>/CeO<sub>2</sub>*”  
Project Seminar at ISUZU Advanced Engineering Center, Isuzu Motors Fujisawa Plant  
2011/07/13, Kanagawa, Japan

#### Oral Presentations in International Conferences (As a Presenter):

1. “*Theoretical investigation on the effect of transition-metal doping on Seebeck coefficient of SiGe alloy*”  
APS March Meeting 2022<sup>\*</sup>  
2022/03/14-18, McCormick Place, Chicago, Illinois, USA
2. “*Influence of transition metal doping on thermoelectric properties of SiGe alloy*”  
PCoMS Symposium & Annual Meeting of Supercomputing Consortium for Computational Materials Science 2021<sup>\*</sup>  
2022/02/14-15, Online via Zoom
3. “*On the doping effect of thermoelectric properties of SiGe alloy from first-principles calculations*”  
CREST Project “Thermal Management” Workshop<sup>\*</sup>

- 2021/12/18, Online via Zoom
4. “Construction of interatomic potential from first-principles database by using genetic algorithm”  
International Webinar on Computational Material Design<sup>‡</sup>  
2021/07/13-15, Online via Zoom
  5. “Effects of transition metal doping on thermoelectric properties of Si<sub>0.5</sub>Ge<sub>0.5</sub> alloy”  
CREST Project “Thermal Control” Workshop<sup>‡</sup>  
2021/03/27, Online via Zoom
  6. “Enhancement of Seebeck coefficient of SiGe alloy by transition metal doping: A first-principles investigation”  
The 168<sup>th</sup> Annual Spring Meeting of the Japan Institute of Metals and Materials<sup>‡</sup>  
2021/03/16-19, Online via Zoom
  7. “Carbon clustering in bcc iron: A kinetic Monte Carlo study”  
PCoMS Symposium & Annual Meeting of Supercomputing Consortium for Computational Materials Science  
2020<sup>‡</sup>  
2021/02/15-16, Online via Zoom
  8. “Cluster variation calculations of pair probabilities in multicomponent alloy: Application to the fcc Cr-Fe-Mn-Ni system”  
The 166<sup>th</sup> Annual Spring Meeting of the Japan Institute of Metals and Materials<sup>†</sup>  
2020/03/17-19, Tokyo Institute of Technology, Tokyo, Japan
  9. “Atomistic kinematics of carbon diffusion and clustering in bcc Fe with point defects”  
APS March Meeting 2020<sup>†</sup>  
2020/03/02-06, Colorado Convention Center, Denver, Colorado, USA
  10. “Carbon diffusion and clustering in bcc iron: A kinetic Monte Carlo study”  
Workshop on Nanotechnology-Driven Topics  
2019/12/10, Osaka University, Osaka, Japan
  11. “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
  12. “Atomistically kinetic simulations of carbon diffusion in  $\alpha$ -Fe with point defect”  
The 32<sup>nd</sup> Meeting on Computational Mechanics of the Japan Society of Mechanical Engineers  
2019/09/16-18, Toyo University, Saitama, Japan
  13. “Cluster Expansion simulations of Fe-C alloys with point defects: Atomic and effective cluster interactions”  
The 164<sup>th</sup> Annual Spring Meeting of the Japan Institute of Metals and Materials  
2019/03/20-22, Tokyo Denki University, Tokyo, Japan
  14. “Diffusion properties of carbon in Fe-C alloy using new Tersoff potential”  
The 31<sup>st</sup> Meeting on Computational Mechanics of the Japan Society of Mechanical Engineers  
2018/11/23-25, Tokushima University, Tokushima, Japan
  15. “Diffusion properties of carbon in  $\alpha$ -Fe”  
PCoMS Symposium & Annual Meeting of Supercomputing Consortium for Computational Materials Science  
2018  
2018/10/22-23, Tohoku University, Miyagi, Japan
  16. “Cluster Expansion Method study on the effective interaction in Fe-C alloys”  
The 163<sup>rd</sup> Annual Fall Meeting of the Japan Institute of Metals and Materials  
2018/09/19-21, Tohoku University, Miyagi, Japan
  17. “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
  18. “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
  19. “New atomic potential of Fe-C binary system for phase transformation of heterogeneous materials”  
The 161<sup>th</sup> Annual Fall Meeting of the Japan Institute of Metals and Materials  
2017/09/06-08, Hokkaido University, Hokkaido, Japan
  20. “Development of interatomic potentials of Fe-C binary system for atomistic materials design of new heterogeneous iron”  
PCoMS Symposium & Annual Meeting of Supercomputing Consortium for Computational Materials Science  
2016  
2016/10/17-18, Tohoku University, Miyagi, Japan
  21. “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
  22. “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

23. “*NO oxidation on CeO<sub>2</sub>-supported Pt<sub>4</sub> cluster: A DFT+U study*”  
Quantum Engineering Design Workshop  
2013/10/25, Osaka University, Osaka, Japan
24. “*NO oxidation on O pre-covered Pt<sub>4</sub>/CeO<sub>2</sub>*”  
OU-TUM Workshop: Trends in Catalysis  
2013/05/16, Osaka University, Osaka, Japan
25. “*Theoretical Investigation on NO oxidation on O pre-covered Pt<sub>4</sub>/CeO<sub>2</sub>*”  
International Workshop on the Theory of Dense Kondo Systems  
2013/03/19-20, Osaka University, Osaka, Japan
26. “*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
27. “*Oxidation of metal and metal oxide systems*”  
Asia Computational Materials Design Workshop  
2011/10/10-12, De La Salle University, Manila, Philippines
28. “*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
29. “*First-principles study on nitric oxide adsorption on metal tape-porphyrines*”  
Asia Computational Materials Design Workshop  
2011/02/15-17, Mahidol University, Bangkok, Thailand
30. “*Adsorption of nitric oxide on metal porphyrin tape*”  
Asia Computational Materials Design Workshop  
2010/12/16-18, Hue University, Hue, Vietnam
31. “*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
32. “*Nitric oxide adsorption effects on metal phthalocyanines*”  
OU-DLSU Academic Research Workshop  
2010/05/27-28, Osaka University, Osaka, Japan
33. “*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
34. “*NO adsorption effects on metal tape-porphyrins*”  
GCOE International Workshop  
2008/11/25-27, Osaka University, Osaka, Japan
35. “*The adsorption of NO on various metal tape-porphyrins*”  
ITB-OU Academic Research Workshop  
2008/06/30, Osaka University, Osaka, Japan
36. “*DFT study on the binding of CO, NO, and O<sub>2</sub> to iron tape-porphyrin*”  
International Workshop on Quantum Simulation 2007  
2007/09/13, Osaka University, Osaka, Japan
37. “*O<sub>2</sub> adsorption effects on electronic properties of Fe tape-porphyrin*”  
International Science and Engineering Workshop  
2007/05/15, Osaka University, Osaka, Japan
38. “*DFT study on O<sub>2</sub> adsorbed Fe tape-porphyrin*”  
The 3<sup>rd</sup> International Workshop on Reactions Involving Oxygen  
2007/05/10, Osaka University, Osaka, Japan
39. “*Study of electronic properties of perovskite BaTiO<sub>3</sub>*”  
The 4<sup>th</sup> Workshop on Simulation & Modeling Physics  
2006/11/22-24, Institute of Physics, Ha-Noi, Vietnam

**Poster Presentations in International Conferences (As a Presenter):**

1. “*Diffusion of carbon in  $\alpha$ -Fe in the presence of vacancy*”  
The 22<sup>th</sup> Asian Workshop on First-Principles Electronic Structure Calculations (ASIAN-22)  
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  $\alpha$ -iron*”  
The 9<sup>th</sup> 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 9<sup>th</sup> 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<sub>n</sub>/CeO<sub>2</sub>(111)*”  
The 54<sup>th</sup> 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 53<sup>rd</sup> Annual Symposium of the Vacuum Society of Japan  
2012/11/14-16, Konan University, Kobe, Japan
  7. “*O<sub>2</sub> adsorption and dissociation on CeO<sub>2</sub>-supported Pt nanoparticles: A DFT+U study*”  
The 5<sup>th</sup> International Symposium on Atomically Controlled Fabrication Technology  
2012/10/22-24, Osaka University, Osaka, Japan
  8. “*Spin effects in metal surface reactions: O<sub>2</sub> on ferromagnetic Pt*”  
AVS 58<sup>th</sup> International Symposium & Exhibition  
2011/10/30-11/04, Nashville Convention Center, Nashville, Tennessee, USA
  9. “*Oxygen dissociation on metal oxide-supported Pt cluster*”  
The 4<sup>th</sup> International Symposium on Atomically Controlled Fabrication Technology  
2011/10/31-11/02, Osaka University, Osaka, Japan
  10. “*Oxygen dissociative adsorption on Pt<sub>4</sub>/CeO<sub>2</sub>(111) surface*”  
The First JSMS Symposium on Multiscale Materials Modeling  
2011/05/23-24, Osaka University, Osaka, Japan
  11. “*Adsorption of nitric oxide on various metal phthalocyanines films by first-principles study*”  
The 3<sup>rd</sup> International Symposium on Atomically Controlled Fabrication Technology  
2010/11/24-26, Osaka University, Osaka, Japan
  12. “*Theoretical study on the oxygen vacancy formation in different platinum-coated CeO<sub>2</sub> surfaces of diesel oxidation catalysts*”  
The 27<sup>th</sup> European Conference on Surface Science  
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<sub>2</sub>(111)*”  
AVS 56<sup>th</sup> 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 21<sup>st</sup> 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<sub>2</sub>*”  
Handai Nanoscience and Nanotechnology International Symposium  
2007/09/26-28, Osaka University, Osaka, Japan
  21. “*DFT study of Jahn-Teller effect in BaTiO<sub>3</sub>*”  
The 3<sup>rd</sup> International Workshop on Nanophysics and Nanotechnology  
2006/12/06-09, Ha-Long, Vietnam
  22. “*Calculation of electronic properties of BaTiO<sub>3</sub> using DFT method*”  
HUS Scientific Conference  
2006/11/11, Ha-Noi University of Science, Ha-Noi, Vietnam
  23. “*First-principles calculation for BaTiO<sub>3</sub>*”  
The 31<sup>st</sup> National Conference on Theoretical Physics  
2006/08/22-25, Hon-Ngu Hotel, Cua-Lo, Nghe-An, Vietnam

## SOCIETAL CONTRIBUTIONS

### Organized Workshops (Overseas):

- The 9<sup>th</sup> Asia Computational Materials Design (CMD®) Workshop  
2017/11/29-12/01, Vietnam-Japan University, Hanoi, Vietnam

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

#### **Academic Society Memberships:**

- Japan Institute of Metals and Materials (since 2017)
- American Physical Society (since 2017)
- 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**

#### **• Prof. Thanh Cong BACH**

Research fields: Condensed Matter Physics, Computational Materials Science, Electronic and Magnetic Properties of Bulk Materials, Many Body Effects  
 Affiliation: Faculty of Physics, VNU University of Science, Vietnam National University (Hanoi)  
 Address: 334 Nguyen Trai Street, Thanh Xuan District, Ha Noi, VIETNAM  
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 E-mail: congbt(at)vnu.edu.vn  
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#### **• Prof. Hideaki KASAI**

Research fields: Condensed Matter Physics at the Nano-Scale, Electronic Properties of Carbon Nanotubes, Hydrogen-Surface Reaction Dynamics, Spintronics Nanomaterials, Nanodevices Design  
 Affiliation: Department of Applied Physics, Graduate School of Engineering, Osaka University  
 Address: 2-1 Yamadaoka, Suita, Osaka 565-0871, JAPAN  
 Telephone: (+81) 06 6879 7857  
 E-mail: kasai(at)dyn.ap.eng.osaka-u.ac.jp  
 ResearchMap URL: <https://researchmap.jp/read0014023>

#### **• Prof. Tetsuo MOHRI**

Research fields: Metallic Physical Properties, Alloy Phase Diagram, Computational Materials Science, First-Principles Calculations, Cluster Expansion/Variation Methods

Affiliation: Professional development Consortium for Computational Materials Scientists, Institute for Materials Research, Tohoku University  
Address: 2-1-1 Katahira, Aobaku, Sendai, Miyagi 980-8577, JAPAN  
Telephone: (+81) 022 215 2327  
E-mail: tmohri(at)imr.tohoku.ac.jp  
ResearchMap URL: <https://researchmap.jp/7000005551>

- **Prof. Yoji SHIBUTANI**

Research fields: Solid Mechanics, Computational Mechanics, Materials Science Size Effects of Solid Mechanics, Multi-Scale Modeling of Defects, Plastic-Physics of Crystalline and Amorphous Materials, Beam-Induced Acoustic Technology  
Affiliation: Division of Mechanical Engineering, Graduate School of Engineering, Osaka University  
Address: 2-1 Yamadaoka, Suita, Osaka 565-0871, JAPAN  
Telephone: (+81) 06 6879 7310  
E-mail: sicutani(at)mech.eng.osaka-u.ac.jp  
ResearchMap URL: <https://researchmap.jp/read0013927>

- **Assoc. Prof. Kazunori SATO**

Research fields: Theoretical Solid State Physics, First-Principles Calculation, Computational Materials Design, Thermoelectric Materials, Machine Learning  
Affiliation: Division of Materials and Manufacturing Science, Graduate School of Engineering, Osaka University  
Address: 2-1 Yamadaoka, Suita, Osaka 565-0871, JAPAN  
Telephone: (+81) 06 6879 7484  
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ResearchMap URL: <https://researchmap.jp/read0076412>

- **Assoc. Prof. Mary Clare ESCAÑO**

Research fields: Surface Science, First-Principles Calculation, Magnetic Multilayers/Alloys, Spintronics, Terahertz  
Affiliation: Research Center for Development of Far-Infrared Region, University of Fukui  
Address: 3-9-1 Bunkyo, Fukui-shi, Fukui 910-8507, JAPAN  
Telephone: (+81) 0776 27 9802  
E-mail: mcescano(at)u-fukui.ac.jp  
ResearchMap URL: <https://researchmap.jp/7000005203>

†No presentation due to COVID-19 pandemic

‡Online presentation due to COVID-19 pandemic

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