CURRICULUM VITAE

NGUYEN TIEN QUANG

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

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Current Position:
Specially-appointed Assistant Professor

Research Fields:
Theoretical and Computational Physics/Chemistry
Computational Materials Science, Condensed Matter Physics

PERSONAL DETAILS

- **Full name:** Nguyen Tien Quang
- **Date of Birth:** 06/10/1982
- **Nationality:** Vietnam
- **Marital Status:** Single
- **Language Proficiency:** Vietnamese (Native), English (Good oral and written communications), Japanese (Basic)

ACADEMIC QUALIFICATIONS

- **Doctor of Philosophy in Engineering**
  Quantum Engineering Design Program
  Department of Applied Physics, Graduate School of Engineering, Osaka University, Japan
  Year of graduation: 2013
  Thesis title: "Theoretical Study on Nitric Oxide Adsorption and Oxidation on Metallo-Macrocycles and Ceria-Supported Platinum Cluster"

- **Master of Engineering**
  Quantum Engineering Design Program
  Department of Applied Physics, Graduate School of Engineering, Osaka University, Japan
  Year of graduation: 2010
  Thesis title: "Adsorption of Nitric Oxide on Metal Porphyrin Tape: The Role of Metal Porphyrin Tape as Sensor in Detecting Nitric Oxide Gas"

- **Master of Science in Theoretical Physics**
  Faculty of Physics, College of Science, Vietnam National University (Hanoi)
  Year of graduation: 2006
  Thesis title: "DFT Study on The Electronic Properties of Perovskite"

- **Bachelor of Science in Physics/Physics Education**
  Teacher Licensure Program
  Faculty of Physics, College of Education, Vietnam National University (Hanoi)
  Year of graduation: 2004
  Thesis title: "Quantum Visualization of Hydrogen Atom"

RESEARCH FIELDS OR SPECIALIZATION

- **Hydrogen Behavior in Iron/Steel:**
  Study of the hydrogen interaction with various defects (vacancies, dislocation, grain boundaries,…) and solutes (carbon, nitrogen, sulfur,…) in iron; and the effects of hydrogen on the mechanical properties of iron/steel for various industrial applications by using first-principles and molecular dynamics methods
- **Diesel Oxidation Catalysts, Three-Way Catalysts:**

Study of oxidation/reduction processes of gases on metal surfaces and metal oxide supported metal clusters for heterogeneous catalysis applications by using DFT+U and molecular dynamics methods

- **Molecular Devices:**
  Study of the electronic and magnetic properties of various metallo-macrocycles (porphyrin, phthalocyanine,...) and their interactions with diatomic gases for sensor applications by using first-principle methods
- **Fuel Cell:**
  Study of oxidation processes on bimetallic surfaces for renewable energy applications by using first-principles and Monte Carlo methods

ACADEMIC/RESEARCH EMPLOYMENT RECORD

- 12/2015-present: (full-time) Assistant Professor in Institute for NanoScience Design, Osaka University, Japan
- 12/2013-12/2015: (full-time) Postdoctoral Researcher at Department of Mechanical Science and Bioengineering, Graduate School of Engineering Science, Osaka University, Japan
- 10/2013-11/2013: (full-time) Postdoctoral Researcher at Department of Applied Physics, Graduate School of Engineering, Osaka University, Japan
- 01/2008-09/2008: (full-time) Visiting Professor at Department of Applied Physics, Graduate School of Engineering, Osaka University, Japan
- 01/2007-12/2007: (full-time) Special Researcher at Department of Applied Physics, Graduate School of Engineering, Osaka University, Japan
- 06/2004-12/2006: (part-time) Teaching Assistant at Faculty of Physics, College of Science, Vietnam National University (Hanoi), Vietnam

INDUSTRIAL RESEARCH EXPERIENCE

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

PATENT

Title: Manufacturing method of chemical substance sensing element, involves including process of selecting material predicted to be suitable for surface modification material of electro-conductive substrate from candidate material
Patent Number: JP2011080798-A
Inventor(s): T. Q. NGUYEN, M. OTONASHI, T. KAWATA, M. YAMANAKA, K. HARA, H. KASAI, H. NAKANISHI
Patent Assignee Name(s) and Code(s): SHARP KK(SHAF-C)
Derwent Primary Accession Number: 2011-E14890 [35]

GRANTS/FELLOWSHIPS

- Japanese Ministry of Education, Culture, Sports, Science and Technology (MEXT) Scholarship under Quantum Engineering Design Program (10/2008-09/2013)
- Japan Student Services Organization (JASSO) Scholarship under Student Exchange Support Program (01-12/2007)

ACQUISITION OF FUNDS

Japan GCOE (Global Center of Excellence TEAM Program):

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

PUBLICATIONS

Books:

1. Mary Clare Sison Escano, Tien Quang Nguyen, Hideaki Kasai, “(Chapter 23) Fundamentals of electronic modification of graphene by Si and H”, Handbook of Graphene Science, Taylor & Francis Group, USA (2016) 351-368, ISBN: 9781466591189

2. Tien Quang Nguyen, Mary Clare Sison Escano, Hideaki Kasai, "(Chapter 6) Porphyrins: Chemistry, Properties and Applications", Handbook of Porphyrins: Chemistry, Properties and Applications, Nova Science Publishers, USA (2012) 229-260, ISBN: 978-1-62081-068-2

Journals:

1. Tien Quang Nguyen, Hajime Kimizuka, Shigenobu Ogata, "Development of an interatomic potential for the Fe-C-H system", Physical Review B (in preparation)
2. Tien Quang Nguyen, Hajime Kimizuka, Shigenobu Ogata, "Hydrogen-Vacancy-Carbon formation in bcc iron: First-principles investigation", Computational Materials Science (submitted)
3. Mary Clare Sison Escano, Tien Quang Nguyen, Hideaki Kasai, "Another way of looking at reactivity enhancement in large area graphene: The role of exchange-splitting from first-principles methods", The Journal of Physical Chemistry C, 119 (2015) 26636
4. Nguyen Hoang Linh, Tien Quang Nguyen, Wilson Agerico Dino, 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
5. Tien Quang Nguyen, Mary Clare Sison Escano, Hiroshi Nakanishi, Hideaki Kasai, Hiroyoshi Maekawa, Kazuo Osumi, Kaoru Sato, "DFT+U study on the oxygen adsorption and dissociation on CeO_2-supported platinum cluster", Applied Surface Science, 288 (2014) 244
6. Tien Quang Nguyen, Allan Abraham Bustria Padama, Mary Clare Sison Escano, Hideaki Kasai, "Theoretical study on The adsorption of NO on metal macrocycles, Metal=Mn,Fe,Co,Ni,Cu,Zn", ECS Transactions, 45 (2013) 91
7. Mary Clare Sison Escano, Tien Quang Nguyen, Hideaki Kasai, "Molecular oxygen adsorption on ferromagnetic platinum", Chemical Physics Letters, 555 (2013) 125
8. Hirofumi Kishi, Ferensa Oemry, Tien Quang Nguyen, Shinichi Kunikata, Hiroshi Nakanishi, Hideaki Kasai, Hiroyoshi Maekawa, Kazuo Osumi, "Study of NO oxidation reaction over the Pt cluster supported on γ-Al_2O_3(111) surface", Current Applied Physics, 12 (2012) S110
9. Mary Clare Sison Escano, Tien Quang Nguyen, Hideaki Kasai, "Analysis of band gap formation in graphene by Si impurities: Local bonding interaction rules", Chemical Physics Letters, 515 (2011) 85
10. Mary Clare Sison Escano, Tien Quang Nguyen, Hideaki Kasai, "Molecular and electronic tuning of Si/CNT hybrid system", Japanese Journal of Applied Physics, 50 (2011) 045101
11. Tien Quang Nguyen, Mary Clare Sison Escano, Hideaki Kasai, "Nitric oxide adsorption effects on metal phthalocyanines", Journal of Physical Chemistry B, 114 (2010) 10017
12. Mary Clare Sison Escano, Tien Quang Nguyen, Hiroshi Nakanishi, Hideaki Kasai, "Another way of looking at bonding on bimetallic surfaces: The role of spin polarization of surface metal d-states", Journal of Physics: Condensed Matter, 21 (2009) 492201
13. Tien Quang Nguyen, Susan Menez Aspera, Hiroshi Nakanishi, Hideaki Kasai, "NO adsorption effects on various functional molecular nanowires", Computational Materials Science, 47 (2009) 111
14. Tien Quang Nguyen, Mary Clare Sison Escano, Reiko Tanaka, Hiroshi Nakanishi, Hideaki Kasai, "The adsorption of NO on various metal tape-porphyrins: A first-principles study", Journal of the Physical Society of Japan, 78 (2009) 014706
15. Mary Clare Sison Escano, Tien Quang Nguyen, Hiroshi Nakanishi, Hideaki Kasai, "Bonding of Pt/Fe overlayer and its effects on atomic oxygen chemisorption from density functional theory study", Surface Science, 602 (2008) 3415
16. Tien Quang Nguyen, Mary Clare Sison Escano, Nobuaki Shimoji, Hiroshi Nakanishi, Hideaki Kasai, "Adsorption of diatomic molecules on iron tape-porphyrin: A comparative study", Physical Review B, 77 (2008) 195307
17. Tien Quang Nguyen, Mary Clare Sison Escano, Nobuaki Shimoji, Hiroshi Nakanishi, Hideaki Kasai, "DFT study on the adsorption of NO on iron tape-porphyrin", Surface and Interface Analysis, 40 (2008) 1082

Proceedings:

1. Mary Clare Sison Escaño, Tien Quang Nguyen, Hiroshi Nakanishi, Hideaki Kasai, "Controlling oxidation reaction on platinum by spin manipulation", Nanotechnology 2012: Electronics, Devices, Fabrication, MEMS, Fluidics and Computational Volume 2, Chapter 9: Modeling and Simulation at the Nanoscale, USA (2012) 645-648, ISBN: 978-1-4665-6275-2
2. Tien Quang Nguyen and Thanh Cong Bach, "First-principles calculation for $BaTiO_3$", Communications in Physics, 17 (2007) 128

PRESENTATIONS

Lectures:

"Computational Materials Design for energy and environmental applications", Asia Computational Materials Design Workshop (06-08/12/2012, Hanoi University of Science, Hanoi, Vietnam) - Lecture for undergraduate students of Faculty of Physics, Hanoi University of Science

Seminars:

"Development of interatomic potentials for modeling of hydrogen and carbon interaction near lattice defects in bcc iron", CAMT Seminars (28/04/2016, Osaka University, Osaka, Japan) - Scientific Seminar at Center for Atomic and Molecular Technologies, Graduate School of Engineering, Osaka University

Oral (International Conferences):

1. "Interatomic potentials for modeling hydrogen and carbon interaction near lattice defects in the Fe-C-H system", International Workshop on Quantum Engineering Design: Materials Design and Realization (24-26/03/2016, Osaka University, Osaka, Japan)
2. "Atomistic Materials Design of New Iron with Highly-Tuned Strength, Ductility and Fracture Toughness: Interatomic Potential Development", PCoMS Kick-off Meeting (26/02/2016, Tohoku University, Tokyo, Japan)
3. "NO oxidation on CeO_2-supported Pt_4 cluster: A DFT+U study", Quantum Engineering Design Workshop (25/10/2013, Osaka University, Osaka, Japan)
4. "First-principles study on NO adsorption and oxidation on metallo-macrocycles and ceria-supported Pt cluster", Mini Symposium on Computational Chemistry for Material Applications (15-16/07/2013, The National University of Malaysia, Selangor, Malaysia) - **Invited talk**
5. "NO oxidation on O pre-covered Pt_4/CeO_2", OU-TUM Workshop: Trends in Catalysis (16/05/2013, Osaka University, Osaka, Japan)
6. "Theoretical Investigation on NO oxidation on O pre-covered Pt_4/CeO_2", International Workshop on The Theory of Dense Kondo Systems (19-20/03/2013, Osaka University, Osaka, Japan)
7. "DFT+U investigation on the adsorption and dissociation of oxygen on Pt-coated Ceria", International Workshop on Current Surface Science Trend (08/11/2012, Osaka University, Osaka, Japan)
8. "Porphyrins and macrocycles: From basics to applications", ECS 221st Meeting (06-10/05/2012, Washington State Convention Center, Seattle, Washington, USA) - **Invited talk**
9. "Oxidation of metal and metal oxide systems", Asia Computational Materials Design Workshop (10-12/10/2011, De La Salle University, Manila, Philippines)
10. "Computational Materials Design case studies: Oxidation of metal/metal oxide systems", International Conference on Quantum Simulations and Design (27-29/09/2011, Max Planck Institute, Dresden, Germany)
11. "First-principles study on nitric oxide adsorption on metal tape-porphyrines", Asia Computational Materials Design Workshop (15-17/02/2011, Mahidol University, Bangkok, Thailand)
12. "Adsorption of nitric oxide on metal porphyrin tape", Asia Computational Materials Design Workshop (16-18/12/2010, Hue University, Hue, Vietnam)
13. "Computational Materials Design of molecular bridge systems for potential applications as nano-electronics devices", International Conference on Core Research and Engineering Science of Advanced Materials & Third International Conference on Nanospintronics Design and Realization (30/05-04/06/2010, Osaka University, Osaka, Japan)
14. "Nitric oxide adsorption effects on metal phthalocyanines", OU-DLSU Academic Research Workshop (27-28/05/2010, Osaka University, Osaka, Japan)
15. "The role of metal porphyrin tape as sensor in detecting NO gas", Asia Computational Materials Design Workshop (26-28/11/2009, Ha-Noi University of Science, Ha-Noi, Vietnam)
16. "NO adsorption effects on metal tape-porphyrins", GCOE International Workshop (25-27/11/2008, Osaka University, Osaka, Japan)
17. "The adsorption of NO on various metal tape-porphyrins", ITB-OU Academic Research Workshop (30/06/2008, Osaka University, Osaka, Japan)
18. "DFT study on the binding of CO, NO, and O_2 to iron tape-porphyrin", International Workshop on Quantum Simulation 2007 (13/09/2007, Osaka University, Osaka, Japan)
19. "O_2 adsorption effects on electronic properties of Fe tape-porphyrin", International Science and Engineering Workshop (15/05/2007, Osaka University, Osaka, Japan)
20. "DFT study on O_2 adsorbed Fe tape-porphyrin", The 3rd International Workshop on Reactions Involving Oxygen (10/05/2007, Osaka University, Osaka, Japan)
21. "Study of electronic properties of perovskite $BaTiO_3$", The 4th Workshop on Simulation & Modeling Physics (22-24/11/2006, Institute of Physics, Ha-Noi, Vietnam)

Poster (International Conferences):

1. "Hydrogen and carbon interactions near lattice defects in bcc iron by combined theoretical methods", 2015 MRS Fall Meeting & Exhibit (29/11-04/12/2015, Boston, Massachusetts, USA)
2. "Atomistic modeling of hydrogen-vacancy-carbon interaction in α-iron", The 9th International Conference on Computational Physics (07-11/01/2015, The National University of Singapore, Singapore)

3. "Hydrogen-vacancy-carbon formation in bcc iron: First-principles study", The 9th General Meeting of Asian Consortium on Computational Materials Science - Virtual Organization (20-22/12/2014, Okinawa Institute of Science and Technology, Okinawa, Japan)
4. "NO oxidation on oxygen pre-covered $Pt_n/CeO_2(111)$", The 54th Annual Symposium of the Vacuum Society of Japan (26-28/11/2013, International Congress Center EPOCHAL, Tsukuba, Japan)
5. "DFT+U investigation on the adsorption and dissociation of oxygen on Pt-coated Ceria", The 53rd Annual Symposium of the Vacuum Society of Japan (14-16/11/2012, Konan University, Kobe, Japan)
6. "O_2 adsorption and dissociation on CeO_2-supported Pt nanoparticles: A DFT+U study", The 5th International Symposium on Atomically Controlled Fabrication Technology (22-24/10/2012, Osaka University, Osaka, Japan)
7. "Spin effects in metal surface reactions: O_2 on ferromagnetic Pt", AVS 58th International Symposium & Exhibition (30/10-04/11/2011, Nashville Convention Center, Nashville, Tennessee, USA)
8. "Oxygen dissociation on metal oxide-supported Pt cluster", The 4th International Symposium on Atomically Controlled Fabrication Technology (31/10-02/11/2011, Osaka University, Osaka, Japan)
9. "Oxygen dissociative adsorption on $Pt_4/CeO_2(111)$ surface", The First JSMS Symposium on Multiscale Materials Modeling (23-24/05/2011, Osaka University, Osaka, Japan)
10. "Adsorption of nitric oxide on various metal phthalocyanines films by first-principles study", The 3rd International Symposium on Atomically Controlled Fabrication Technology (24-26/11/2010, Osaka University, Osaka, Japan)
11. "Theoretical study on the oxygen vacancy formation in different platinum-coated CeO_2 surfaces of diesel oxidation catalysts", The 27th European Conference on Surface Science (29/08-03/09/2010, Martiniplaza, Groningen, Kingdom of The Netherlands)
12. "Theoretical study on the adsorption of NO on metal phthalocyanines for biosensor application", International Conference on Core Research and Engineering Science of Advanced Materials & Third International Conference on Nanospintronics Design and Realization (30/05-04/06/2010, Osaka University, Osaka, Japan)
13. "DFT study of oxygen vacancy formation in a diesel oxidation catalyst: $Pt/CeO_2(111)$", AVS 56th International Symposium & Exhibition (08-13/11/2009, San Jose Convention Center, San Jose, California, USA)
14. "A DFT study on adsorption of NO on various functional molecular nanowires", Japanese Physical Society Meeting (25-28/09/2009, Kumamoto University, Kumamoto, Japan)
15. "Theoretical study on interaction of NO with metal tape-porphyrins", First International Symposium on Atomically Controlled Fabrication Technology (16-17/02/2009, Osaka University, Osaka, Japan)
16. "DFT study on the adsorption of NO on various metal tape-porphyrins", International Symposium on Surface Science and Nanotechnology (09-13/11/2008, Waseda University, Tokyo, Japan)
17. "Adsorption of NO on various metal tape-porphyrins by first-principles study", International Conference on Quantum Simulators and Design 2008 (31/05-03/06/2008, National Museum of Emerging Science and Innovation, Tokyo, Japan)
18. "The adsorption of diatomic molecules on iron tape-porphyrin: A comparative study", International 21st Century COE Symposium on Atomistic Fabrication Technology 2007 (15-17/10/2007, Osaka University, Osaka, Japan)
19. "A theoretical study on the interaction between iron tape-porphyrin and CO, NO, and O_2", Handai Nanoscience and Nanotechnology International Symposium (26-28/09/2007, Osaka University, Osaka, Japan)
20. "DFT study of Jahn-Teller effect in $BaTiO_3$", The 3rd International Workshop on Nanophysics and Nanotechnology (06-09/12/2006, Ha-Long, Vietnam)
21. "Calculation of electronic properties of $BaTiO_3$ using DFT method", HUS Scientific Conference (11/11/2006, Ha-Noi University of Science, Ha-Noi, Vietnam)
22. "First-principles calculation for $BaTiO_3$", The 31st National Conference on Theoretical Physics (22-25/08/2006, Hon-Ngu Hotel, Cua-Lo, Nghe-An, Vietnam)

COMPUTER SKILLS AND OUTPUTS

Skills:

- Operating systems: Windows, Mac OS X, Linux (Fedora, Ubuntu, SuSE, CentOS)
- Programing languages: Very experienced in FORTRAN, MATLAB; knowledgable in C/C++, Python, MPI, Shell-scripts, Mathematica, HTML, Markdown, LaTeX
- Office applications: MS Office, Apple iWork, OpenOffice
- Simulation packages: Dacapo, VASP, STATE-Senri, AkaiKKR, LAMMPS
- Visualization softwares: GNUplot, VESTA, CrystalMaker, VMD, Ovito, AtomEye

Outputs:

- FORTRAN program for generating interatomic potentials for ternary systems using Genetic Algorithm
- FORTRAN program for Monte Carlo simulation of magnetic properties of bimetallic surfaces

- FORTRAN utilities for analysis/manipulating output data of Vienna Ab-initio Simulation Program
- MATLAB Graphic User Interface program for Visualizing Hydrogen Atomic Orbitals

OUTREACH

Organizer of:

- Asia Computational Materials Design Workshop, Hanoi University of Science, Hanoi, Vietnam (6-8/12/2012)
- HUS-OU-UBC International Workshop on Quantum Design and Realization, Osaka University, Japan (27-28/02/2012)
- Asia Computational Materials Design Workshop, Saigon University, Ho Chi Minh City, Vietnam (09-11/12/2011)
- Asia Computational Materials Design Workshop, Mahidol University, Bangkok, Thailand (15-17/02/2011)
- Asia Computational Materials Design Workshop, Hue University, Hue, Vietnam (16-18/12/2010)
- HUS-OU-BBK Scientific Workshop, Osaka University, Japan (22/11/2010)
- Asia Computational Materials Design Workshop, Hanoi University of Science, Hanoi, Vietnam (16-18/12/2009)
- HUS-OU International Workshop on Quantum Simulation, Osaka University, Japan (12/09/2008)
- HUS-OU International Workshop on Quantum Simulation, Osaka University, Japan (13/09/2007)

MEMBERSHIPS

- Materials Research Society
- Vacuum Society of Japan
- Physical Society of Japan
- American Vacuum Society
- Vietnamese Theoretical Physical Society

JOURNAL REFEREEING

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

OTHERS

- Tutor for Asia CMD Workshop
- Research supervisions/guidance for younger students
- Setting up computational facilities for Asia CMD Workshop
- Research group's computer cluster system management
- Quantum Engineering Design Course official website establishment and maintenance