

TANGLAW ROMAN

CURRICULUM VITAE

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CORE INTERESTS

- Renewable resources, clean energy technology and sustainable materials
- Electronic structure, excitation, exchange and correlation
- High-performance computing for ab initio molecular dynamics
- Quantum computing algorithms for chemistry and condensed matter physics
- Linux and open-source solutions
- Education – physics, physical chemistry, quantum chemistry, materials engineering
- History and philosophy of Science

RESEARCH AND TEACHING EXPERIENCE

Research Associate & Lecturer

*The University of Sydney Nano Institute (Sydney Nano)
and the Condensed Matter Theory Group, School of Physics
The University of Sydney, New South Wales, Australia*

November 2019 – present

- Research areas:
 - Resolving mechanisms of CO₂ reduction on emerging nanocatalysts
- Auxiliary Supervisor to postgraduate research students (PhD and MS students)
- Courses taught:
 - [PHYS3036](#) Condensed Matter and Particle Physics

Research Fellow & Lecturer

*Condensed Matter Physics, School of Mathematics and Physics
The University of Queensland, Brisbane, Australia*

March 2019 – October 2019

- Research areas:
 - Superexchange interactions in metal-organic spinchains for quantum communication
- Supervised the capstone research projects of two undergraduate students ([PHYS3900](#))
- Courses taught:
 - [PHYS4030](#) Condensed Matter Physics: Electronic properties of crystals (30% role) – Honours
 - [PHYS7033](#) Condensed Matter Physics: Electronic properties of crystals (30% role) – Masters

Research Fellow

*Centre for Theoretical and Computational Molecular Science
Australian Institute for Bioengineering & Nanotechnology (AIBN)
The University of Queensland, Brisbane, Australia*

November 2017 – April 2019

- Research areas:
 - Transport properties of polymers and superionic conductors under equilibrium and non-equilibrium conditions
 - Electrochemical energy storage technology
- Coordinator, seminars of the Centre for Theoretical and Computational Molecular Science (joint monthly seminars of computational materials groups University of Queensland, Queensland University of Technology, and Griffith University)

Academic Staff Member & Research Systems Administrator

*Institute of Theoretical Chemistry, Faculty of Natural Sciences
Ulm University (Universität Ulm), Ulm, Germany*

August 2010 – October 2016

- Research areas:

- Dynamic structure of solid-liquid interfaces
- Modified electrode work functions arising from adsorption-induced surface dipoles
- Anion coverages on electrodes
- Electron transfer at the electrochemical interface
- Managed all computing facilities, network file systems and Linux workstations of the Institute of Theoretical Chemistry
- Managed projects at the Leibniz Supercomputing Centre
- Handled tutorials in Quantum Mechanics for undergraduate Chemistry students

Research Assistant Professor

*Division of Precision Science & Technology and Applied Physics, Graduate School of Engineering
Osaka University, Osaka, Japan (大阪大学大学院工学研究科・応用物理学専攻)*

April 2010 – June 2010

- Research areas:
 - Reversible hydrogen reactions for next-generation battery technology and oxygen dissociative adsorption dynamics
- Lectured on solid state physics to graduate students

Research Scientist

*Department of Applied Physics, Graduate School of Engineering
Osaka University, Osaka, Japan*

May 2004 – March 2005

- Research areas:
 - Computational analysis of strong adhesion of thermoplastics with metals
 - Structural, electronic and magnetic properties of modified carbon nanotubes
- Organized the Osaka University – De La Salle University Science Research Workshops and established its conference proceedings

Assistant Instructor

*Department of Physics, College of Science
De La Salle University, Manila, Philippines*

October 2003 – April 2004

- Research areas:
 - Multi-instrument determination of properties, spatial and temporal distribution of urban atmospheric aerosols
- Lectured on general physics and supervised laboratory work for science, engineering and liberal arts undergraduate students

HIGHER EDUCATION

Doctor of Philosophy in Engineering

*Precision Science Technology & Applied Physics
Osaka University, Osaka, Japan*

April 2007 – March 2010

Dissertation: *Structural and dynamical properties of hydrogen in graphene and platinum surface systems* ([online](#))

Master of Engineering

*Applied Physics
Osaka University, Osaka, Japan*

April 2005 – March 2007

Thesis: *Toward a hydrogen economy: high-uptake hydrogenation and quantum migration*

Bachelor of Science, Magna cum laude

*Physics with specialization in Computer Electronics/Applications
De La Salle University, Manila, Philippines and National University of Singapore, Singapore*

June 1999 – September 2003

January 2002 – December 2002 (coursework in Singapore – 29 lecture and lab units)

Thesis: *Retrieval of cloud and aerosol depolarization and optical properties using two-wavelength multi-angle lidar sensing*

RESEARCH HIGHLIGHTS

- 50 peer-reviewed journal articles
- Including top-tier journals such as *Physical Review Letters* and *Advanced Materials*
- 67 co-authors
- h-index: 19 (Google)
- Citations: 1066 (Google)
- 7 publications with more than 50 citations
- 1 book chapter
- Reviewer for journals including *Nature Communications* and *Advanced Materials*

PUBLICATIONS

Book chapters

1. T. Roman and H. Kasai, *Structural and electronic properties of hydrogenated graphene*, Carbon Nanomaterials for Gas Adsorption, edited by M.L. Terranova, S. Orlanducci and M. Rossi (2012), Pan Stanford Publishing/CRC Press

Peer-reviewed journal articles (with external links)

1. S. Sakong, D. Mahlberg, T. Roman, M. Li, M. Pandey, A. Groß, *Influence of local inhomogeneities and the electrochemical environment on the oxygen reduction reaction on Pt-based electrodes: A DFT study*, ACS Catalysis, submitted.
2. A. Baktash, J. Reid, T. Roman, D.J. Searles, *Diffusion of lithium ions in lithium-argyrodite solid state electrolytes from equilibrium and nonequilibrium molecular dynamics simulations*, NPJ Computational Materials (2020), accepted ([arXiv](#)).
3. A. Baktash, J. Reid, Q. Yuan, T. Roman, D.J. Searles, *Shaping the future of solid-state electrolytes through computational modeling*, *Advanced Materials* (2020), **32**, 1908041
4. A.H. Farokh Niaei, T. Roman, T. Hussain, D.J. Searles, *A computational study on the adsorption of sodium and calcium on edge-functionalized graphene nanoribbons*, *J. Phys. Chem. C* (2019), **123**, 14895-14908
5. F. Gossenberger, T. Roman and A. Groß, *Hydrogen and halide co-adsorption on Pt(111) in an electrochemical environment: a computational perspective*, *Electrochim. Acta* **216** (2016) 152-159.
6. J.M. Fischer, D. Mahlberg, T. Roman and A. Groß, *Water adsorption on bimetallic PtRu/Pt(111) surface alloys*, *Proc. R. Soc. A* **472** (2016) 20160618 (and its [issue cover](#))
7. T. Roman* and A. Groß, *Polymorphism of water in two dimensions*, *J. Phys. Chem. C* **120** (2016) 13649-13655
8. F. Gossenberger, T. Roman and A. Groß, *Equilibrium coverage of halides on metal electrodes*, *Surf. Sci.* **631** (2015) 17
9. N.G. Hörmann, M. Jäckle, F. Gossenberger, T. Roman, K. Forster-Tonigold, M. Naderyan, S. Sakong and A. Groß, *Some challenges in the first-principles modeling of structures and processes in electrochemical energy storage and transfer*, *J. Power Sources* **275** (2015) 531-538
10. W. Brenig and T. Roman, *Graphene and graphite, low-temperature catalysts producing weakly excited hydrogen molecules*, *Chem. Phys.* **439** (2014) 117
11. P. Schnäbele, R. Korytar, A. Bagrets, T. Roman, A. Groß and F. Evers, *Ab initio transport calculations for single-atom copper junctions in the presence of hydrogen chloride*, *J. Phys. Chem.* **118** (2014) 28252-28257
12. A. Groß, F. Gossenberger, X. Lin, M. Naderian, S. Sakong and T. Roman, *Water structures at metal electrodes studied by ab initio molecular dynamics simulations*, *J. Electrochem. Soc.* **161** (2014) E3015
13. T. Roman, F. Gossenberger, K. Forster-Tonigold and A. Groß, *Halide adsorption on close-packed metal electrodes*, *Phys. Chem. Chem. Phys.* **16** (2014) 13630
14. F. Gossenberger, T. Roman, K. Forster-Tonigold and A. Groß, *Change of the work function of platinum electrodes induced by halide adsorption*, *Beilstein J. Nanotechnol.* **5** (2014) 152
15. T. Roman and A. Groß, *Structure of water layers on hydrogen-covered Pt electrodes*, *Catal. Today* **202** (2013) 183
16. T. Roman* and A. Groß, *Periodic density-functional calculations on work function change induced by adsorption of halogens on Cu(111)*, *Phys. Rev. Lett.* **110** (2013) 156804
17. P. Quaino, N. Luque, G. Soldano, R. Nazmutdinov, E. Santos, T. Roman, A. Lundin, A. Groß and W. Schmickler, *Solvated protons in density functional theory - a few examples*, *Electrochim. Acta* **105** (2013) 248
18. T. Roman, H. Nakanishi and H. Kasai, *High-uptake graphene hydrogenation: a computational perspective*, *J. Phys: Condens. Matter* **21** (2009) 474219

19. T. Roman, H. Nakanishi and H. Kasai, *Halogen-assisted copper atom abstraction: a computational perspective*, *Jpn. J. Appl. Phys.* **48** (2009) 095501
20. T. Roman, H. Nakanishi, H. Kasai, K. Nobuhara, T. Sugimoto and K. Tange, *Stability of three-hydrogen clusters on graphene*, *J. Phys. Soc. Jpn.* **78** (2009) 035002
21. M. David, R. Muhida, T. Roman, H. Nakanishi, W.A. Diño, H. Kasai, F. Takano, H. Shima and H. Akinaga, *First principles calculations-based model for the reactive ion etching of metal oxide surfaces*, *Vacuum* **83** (2009) 599
22. T. Roman, H. Nakanishi and H. Kasai, *Coadsorbed H and CO interaction on platinum*, *Phys. Chem. Chem. Phys.* **10** (2008) 6052
23. N. Ozawa, T. Roman, M. David, H. Kishi and H. Kasai, *Modeling the reactive ion etching process for the CoO(001) surface via first principles calculations*, *J. Phys: Condens. Matter* **20** (2008) 355006
24. F. Takano, H. Shima, H. Muramatsu, Y. Kokaze, Y. Nishioka, K. Suu, H. Kishi, N. B. Arboleda, Jr., M. David, T. Roman, H. Kasai and H. Akinaga, *Reactive ion etching process of transition-metal oxide for resistance random access memory device*, *Jpn. J. Appl. Phys.* **47** (2008) 6931-6933
25. H. Kishi, N. Ozawa, M. Y. David, T. Roman, N. B. Arboleda Jr., W.A. Diño, H. Nakanishi, H. Kasai, F. Takano, H. Shima and H. Akinaga, *Density functional theory based evaluations of the reactive ion etching process model for TiO₂(anatase) thin film*, *J. Vac. Soc. Jpn.* **51** (2008) 397-400
26. T. Roman, W.A. Diño, H. Nakanishi, H. Kasai, K. Nobuhara, T. Sugimoto and K. Tange, *Identifying hydrogen atoms on graphite*, *J. Phys. Soc. Jpn.* **76** (2007) 114703
27. T. Roman, W.A. Diño, H. Nakanishi, H. Kasai, T. Sugimoto and K. Tange, *Hydrogen pairing on graphene*, *Carbon* **45** (2007) 218-220
28. M. David, R. Muhida, T. Roman, S. Kunikata, W.A. Diño, H. Nakanishi, H. Kasai, F. Takano, H. Shima and H. Akinaga, *Applying computational nanomaterials design to the reactive ion etching of NiO thin films —a preliminary investigation*, *J. Phys: Condens. Matter* **19** (2007) 365210
29. E.S. Dy, T. Roman, Y. Kubota, K. Miyamoto and H. Kasai, *Exploring haem-based alternatives for oxygen reduction catalysis in fuel cells*, *J. Phys.: Condens. Matter* **19** (2007) 445010
30. N. Ozawa, N. B. Arboleda Jr, T. Roman, W.A. Diño, H. Nakanishi and H. Kasai, *Quantum states of a hydrogen atom motion on the Pd(111) surface and in the subsurface*, *J. Physics: Condens. Matter* **19** (2007) 365214
31. N. Ozawa, N. B. Arboleda Jr., T. Roman, W.A. Diño, H. Nakanishi and H. Kasai, *Potential energy of hydrogen atom motion on Pd(111) surface and in subsurface: a first principles calculation*, *J. Appl. Phys.* **101** (2007) 123530
32. N. Ozawa, T. Roman, H. Nakanishi, W.A. Diño and H. Kasai, *Quantum states of a hydrogen atom adsorbed on Cu(100) and (110) surfaces*, *Phys. Rev. B* **75** (2007) 115421
33. M. David, T. Roman, W.A. Diño, H. Nakanishi, H. Kasai, N. Ando and M. Naritomi, *Nanoscale understanding of the adhesion of polybutylene terephthalate on aluminum*, *Surf. Sci.* **601** (2007) 5241-5245
34. S. Matsumoto, W.A.T. Diño, M.Y. David, R. Muhida, T.A. Roman, S. Kunikata, F. Takano, H. Akinaga and H. Kasai, *Design of reactive ion etching process based on ab-initio calculation - The first step*, *J. Vac. Soc. Jpn.* **50** (2007) 437-439
35. M. David, T. Roman, W.A. Diño, H. Nakanishi, H. Kasai, N. Ando and M. Naritomi, *Polybutylene Terephthalate Adhesion on Metals: A Density Functional Theory Investigation*, *J. Vac. Soc. Jpn.* **49** (2006) 433-436
36. T. Roman, H. Nakanishi, W.A. Diño and H. Kasai, *Hydrogen atom quantum migration on platinum*, *e-J. Surf. Sci. Nanotechnol.* **4** (2006) 619-623
37. T. Roman, W.A. Diño, H. Nakanishi, H. Kasai, T. Sugimoto and K. Tange, *Realizing a carbon-based storage material*, *Jpn. J. Appl. Phys.* **45** (2006) 1765-1767
38. T. Roman, W.A. Diño, H. Nakanishi and H. Kasai, *Amino acid adsorption on single-walled carbon nanotubes*, *Eur. Phys. J. D*, **38** (2006) 117-120
39. T. Roman, W.A. Diño, H. Nakanishi and H. Kasai, *Amino acid adsorption effects on nanotube electronics*, *J. Vac. Soc. Jpn* **49** (2006) 46-48
40. T. Roman, W.A. Diño, H. Nakanishi and H. Kasai, *Glycine adsorption on single-walled carbon nanotubes*, *Thin Solid Films*, **509** (2006) 218-222
41. N. Ozawa, T. Roman, H. Nakanishi and H. Kasai, *Quantum states of hydrogen (H, D, T) atoms on Cu(100)*, *Surf. Sci.* **600** (2006) 3550-3554
42. M. David, T. Roman, H. Nakanishi, H. Kasai, N. Ando and M. Naritomi, *A density functional theory-based investigation of adhesion of polybutylene terephthalate on aluminum*, *Thin Solid Films* **509** (2006) 215-217
43. M. David, T. Roman, W.A. Diño, H. Nakanishi, H. Kasai, N. Ando and M. Naritomi, *Polybutylene terephthalate on metals: a density functional theory and cluster models investigation*, *J. Phys. Cond. Matt.*, **18** (2006) 1137-1142
44. T. Roman, W.A. Diño, H. Nakanishi, H. Kasai, Y. Miyako, N. Ando and M. Naritomi, *Examining*

- poly(phenylene sulfide) adhesion using cluster models*, *J. Vac. Soc. Jpn.* **48** (2005) 235-237
45. R. Muhida, A. Susanto, T. Kishi, T. Roman, H. Nakanishi and H. Kasai, *Density functional calculations for H₂ adsorption on Fe(OH)₃ by considering molecular orientation*, *J. Vac. Soc. Jpn.* **48** (2005) 199-201
 46. M. Kisaku, M. M. Rahman, T. Roman, W.A. Diño, H. Nakanishi and H. Kasai, *Diameter size-dependent magnetic and electronic properties of single-walled carbon nanotubes with Fe nanowires*, *Jpn. J. Appl. Phys.* **44** (2005) 882-888
 47. M.M. Rahman, M. Kisaku, T. Kishi, T. Roman, W.A. Diño, H. Nakanishi and H. Kasai, *Electric and magnetic properties of Co-filled carbon nanotube*, *J. Phys. Soc. Jpn.* **74** (2005) 742-745
 48. T. Roman, W.A. Diño, H. Nakanishi, H. Kasai, Y. Miyako and M. Naritomi, *PPS-metal adhesion: a density functional theory-based study*, *Solid State Commun.* **132** (2004) 405-408
 49. R. Muhida, M.M. Rahman, M. Tsuda, T. Roman, W.A. Diño, H. Nakanishi and H. Kasai, *Change of magnetic properties of benzenes in multiple-decked sandwich clusters: Mn_n(C₆H₆)_{n+1} (n = 1,2)*, *J. Physics: Condens. Matter* **16** (2004) S5749-S5753
 50. M.C.D. Galvez, E.A. Vallar, E.B. Bangsal, E.P. Macalalad and T. Roman, *Multi-angle LIDAR sensing of traffic aerosols in Manila*, Proceedings of the 22nd International Laser Radar Conference, *European Space Agency (ESA) Publications SP-561* (2004) 545
 51. E.A. Vallar, M.C.D. Galvez, J.C.Q. Uy, E.P. Macalalad, T. Roman and E.B. Bangsal, *Multi-instrument particulate matter characterization during the 2004 New Year celebration in Manila (14°33.978' N; 120°59.523' E)*, Proceedings of the 22nd International Laser Radar Conference, *European Space Agency (ESA) Publications SP-561* (2004) 549

* Corresponding author

Theses

1. *Structural and dynamical properties of hydrogen in graphene and platinum surface systems*, PhD dissertation, Osaka University (2010) ([online](#))
2. *Toward a hydrogen economy: high-uptake hydrogenation and quantum migration*, Masters thesis, Osaka University (2007)
3. *Retrieval of cloud and aerosol depolarization and optical properties using two-wavelength multi-angle lidar sensing*, Bachelors thesis, De La Salle University (2003)

Other publications

1. T. Roman, M. Jäckle, *Role of the Exchange Mechanism in Lithium Self-Diffusion Processes*, High Performance Computing in Science and Engineering (2014), edited by S. Wagner, A. Bode, H. Satzger and M. Brehm ([online](#))
2. T. Roman, J. Kucera, K. Tonigold, X. Lin, D. Künzel, A. Groß, *Structures and processes at metal-liquid interfaces*, High Performance Computing in Science and Engineering (2012), edited by S. Wagner, A. Bode, H. Satzger and M. Brehm ([online](#))
3. T. Roman, H. Kishi, H. Nakanishi, H. Kasai, *Halogen-based copper etching dynamics: potential energy surfaces*, Proceedings of the Ninth OU-DLSU Science Research Workshop (2008), ISBN 971555512-8
4. E. B. Bangsal, T.A. Roman, E.P. Macalalad, J.C. Uy, G. Bagtasa, M. Dela Cruz, H.W. Chua, E.A. Vallar, and M.C.D. Galvez, *Elemental Composition of Airborne Fine Particulate Matter during the 2004, 2005, 2006 and 2007 New Year Celebrations in Manila*, Proceedings of the Ninth OU-DLSU Academic Research Workshop (2008), ISBN 971555512-8
5. T. Roman, W.A. Diño, H. Nakanishi, H. Kasai, T. Sugimoto and K. Tange, *Graphite utilization in hydrogen storage: a computational perspective*, *Intl. J. Energy, Environment and Economics* **14** (2007) 163-171
6. T. Roman, H. Nakanishi, and H. Kasai, *On fuel cells: H-Pt(111) revisited*, Proceedings of the Seventh OU-DLSU Academic Research Workshop (2007), ISBN 971555512-8
7. T. Roman, H. Nakanishi and H. Kasai, *H—CO interaction on Pt: potential energy surface*, Proceedings of the Fifth OU-DLSU Science Research Workshop (2006), ISBN 971555512-8
8. M. David, T. Roman, W.A. Diño, H. Nakanishi, H. Kasai, N. Ando and M. Naritomi, *A Study on the Adhesion of Polybutylene Terephthalate on Aluminum*, Proceedings of the Fourth OU-DLSU Science Research Workshop (2006), ISBN 971555512-8
9. E.B. Bangsal, T.A. Roman, E.P. Macalalad, J.C. Uy, E.A. Vallar, and M.C.D. Galvez, *Elemental Composition of Airborne Fine Particulate Matter During The 2004 New Year Celebration in Manila*, Proceedings of the Third OU-DLSU Science Research Workshop (2006), ISBN 971555512-8
10. T. Roman, W. A. Diño, H. Nakanishi, H. Kasai, T. Sugimoto and K. Tange, *Controlling Graphite for Hydrogen Storage*, Proceedings of the Third OU-DLSU Science Research Workshop (2006), ISBN 971555512-8

EXTERNAL ACTIVITIES AND AFFILIATIONS

Active peer reviewer in scientific journals

- *Nature Communications* (Nature)
- *NPJ Computational Materials* (Nature)
- *Advanced Materials* (Wiley)
- *The Journal of Physical Chemistry* (American Chemical Society)

Professional organizations

Australian Institute of Physics (AIP), *Member*

Royal Australian Chemical Institute (RACI), *Member*

REFERENCES

Available upon request.

LINKS

- [ORCiD](#)
- [LinkedIn](#)

Sydney, Australia, 24 September 2020

Tanglaw Roman