Takashi Tsuchimochi

Associate Professor
Graduate School of System Informatics, Kobe University
1-1 Rokkodai-cho, Nada-ku, Kobe 657-8501, Japan
tsuchimochi@gmail.com
(as of 12/26/2022)

EDUCATION

Bachelor of Science, 2007
Waseda University, Tokyo

Doctor of Philosophy, 2012
Rice University, TX

HONORS AWARDS

Waseda Card Scholarship (Waseda University), 2004-2006
Ajinomoto Scholarship, 2006
Best Thesis Award (Waseda University), 2007
Stephen C. Hoffman Award (Rice University), 2009
Harry B. Weiser Research Award (Rice University), 2011
Travel Award (The Seventh Congress of the International Society for Theoretical Chemical Physics, Tokyo), 2011
Lodieska Stockbridge Vaughn Fellowship (Rice University), 2011-2012
Young Scientist Award, Japan Society for Molecular Science, 2019
Young Scientist Award, Japan Society of Theoretical Chemistry, 2020
Maenosono Excellent Paper Award, Kobe University, 2022
Young Investigator Award, Kobe University, 2022

PROFESSIONAL EXPERIENCE

Associate Professor (2020 – Present)
Graduate School of System Informatics, Kobe University, Kobe

PRESTO Researcher (Concurrent) (2020 – Present)
Japan Science and Technology Agency, Saitama

Lecturer (Full-time) (2018 – 2020)
Graduate School of System Informatics, Kobe University, Kobe

Research assistant professor (2016 – 2018)
Graduate School of Science, Technology, and Innovation, Kobe University, Kobe

Research assistant professor (2015 – 2016)
Graduate School of System Infromatics, Kobe University, Kobe

Postdoctoral associate (2012 – 2015)
Department of Chemistry, Massachusetts Institute of Technology, Cambridge, MA

Research assistant (2008 – 2012)

Department of Chemistry, Rice University, Houston, TX

Research assistant (2007)
Waseda Institute for Advanced Study, Tokyo

GRANTS-IN-AID

KAKENHI Young Scientist (B), 2017-2020, ¥4,940,000. Developments and applications of novel electronic structure theories for degenerate systems with an accurate description of spin

KAKENHI Young Scientist, 2020-2023, ¥4,160,000. Developments of novel methods for excited states toward understanding mechanisms of excitons in organic molecular aggregates

JST PRESTO, 2020-2024, ¥28,000,000. Development of a comprehensive quantum algorithm for diverse electronic structures

---

REFEREE ACTIVITY

Journal of Chemical Theory and Computation
Journal of Chemical Physics
Journal of Physical Chemistry C
Chemical Science
International Journal of Quantum Chemistry

TEACHING EXPERIENCE

CHEM153 Honors Chemistry (Laboratory TA), Rice University, Fall 2007
CHEM124 General Chemistry (Laboratory TA), Rice University, Spring 2008
CHEM310 Physical Chemistry (TA with Profs. Stephan Link and Christy Landes), Rice University, Fall 2009

Interdisciplinary Experiment B1, B2, Kobe University, 3Q-4Q 2018 – 2021
Computation of Micro-mechanical Systems, Kobe University, 3Q 2018 –2020, 3Q-4Q 2021
Computational Physical Chemistry, Kobe University, 3Q-4Q 2019 – 2021
Introduction to Computer Literacy, Kobe University, 1Q 2021 – 2022

RESEARCH INTERESTS

- Machine learning for predicting/unraveling functionality of materials.
- Development of methodologies for describing static correlations in strongly correlated systems for both ground and excited states.
- Quantum computing for Quantum Chemistry and other subjects (dynamical correlations excited states by classical-quantum hybrid algorithms).
- Application of first-principle approaches to photochemistry and electrochemistry toward next-generation energy sources.
- Investigation of new materials that exhibit unusual spin characters, including single molecule magnets.

PRESENTATIONS

July 2019: *Ionization potentials for multi-reference systems via post-PHF: Extended Koopmans' Theorem*,
9th Molecular Quantum Mechanics Conference, Heidelberg, Germany (poster)

June 2018: *Orbital-invariant coupled-cluster theory combined with spin-projection*,
16th International Congress of Quantum Chemistry, Menton, France (poster)

August 2017: *Towards accurate description of weak and strong correlations via spin-projection*,
11th Triennial Congress of the World Association of Theoretical and Computational Chemists, Munich, Germany (poster)

March 2016: *Black-box and highly accurate approach to dynamic and static electron correlation based on spin projection*,
the 251st ACS National Meeting, San Diego, California (oral)

May 2015: *Development and implementation of time-dependent projected Hartree-Fock and applications to excited states in degenerate molecules.*,
18th Theoretical Chemistry Symposium, Osaka, Japan (oral in Japanese)

March 2015: *Time-dependent projected Hartree-Fock for degenerate excited states*,
249th ACS National Meeting & Exposition, Denver, Colorado (oral)

September 2014: *Extended Second-Order Møller-Plesset Perturbation Theory*,
8th Annual Meeting of Japan Society for Molecular Science, Hiroshima, Japan (oral in Japanese)

July 2014: *Extended Møller-Plesset perturbation theory*,
American Conference on Theoretical Chemistry 2014, Telluride, Colorado (poster)

June 2013: *Restricted Open-Shell Kohn-Sham Theory for Organic Molecular Systems: Application to Stokes Shifts*,
7th Molecular Quantum Mechanics 2013, Lugano, Switzerland (poster)

September 2011: *Generalization of Constrained Unrestricted Mean-Field Methods for Controlling Spin-Contamination: Application to Singlet-Triplet Splitting Energies*,
7th Congress of the International Society for Theoretical Chemical Physics, Tokyo, Japan (oral)

June 2011: *Constrained Active Space Unrestricted Mean-Field Methods for Controlling Spin-Contamination: Application to Singlet-Triplet Splitting Energies*,
Pan American Advanced Studies Institute on "ELECTRONIC PROPERTIES OF COMPLEX SYSTEMS", Cartagena, Colombia (poster)

March 2011: *Constrained Active Space Unrestricted Mean-Field Approaches for Controlling Spin-Contamination*,
2011 American Physical Society March Meeting, Dallas, Texas (oral)

March 2007: *Cost effective calculations of core-excitation energies using Sakurai-Sugiura projection method*,
87th Annual Meeting of The Chemical Society of Japan, Osaka, Japan (oral in Japanese)

November 2006: *Hybrid functional for core- and Rydberg-excitation calculations II*,
2006 Annual Meeting of Society of Computer Chemistry Japan, Hakodate, Japan (poster in Japanese)

INVITED TALKS

January 2022: *Hybrid Classical-Quantum Algorithms for Quantum Chemistry*, China-Japan-Korea tripartite Workshop on Theoretical and Computational Chemistry (CJK-WTCC), Virtual conference

December 2021: *Quantum spin-projection in variational quantum computing*, Pacifichem 2020, Honolulu, Hawaii

November 2021: *Understanding the photocatalytic mechanism in the Z-scheme of BiVO4 and few-layer black phosphorus*, EU-Japan workshop on HPC-based material sciences (Virtual Conference)

September 2021: *Systematic Approach to Electron Correlation via Spin-symmetry Breaking and Restoration*, The 15th Annual Meeting of Japan Society for Molecular Science, Sapporo (Virtual Conference) (Japanese)

May 2021: *Systematic developments of novel wave function theory based on symmetry-breaking and restoration*, The 23rd Annual Meeting of Japan Society of Theoretical Chemistry (Virtual Conference) (Japanese)

June 2020: *Recovering spin-symmetry in classical and quantum computers*, Low-scaling and Unconventional Electronic Structure Techniques Conference (LUEST) 2020, Telluride, Colorado (Virtual Conference)

December 2019: *Symmetry-breaking in a wave function and entanglement*, QIQB Symposium, Osaka University

October 2019: *Second-Order Perturbation Theory with Spin-Projected Hartree-Fock*, APATCC 2019, Sydney, Australia

August 2019: *Electronic structure calculations on transition metal complexes with the correct spin picture*, Workshop on Computational Biological Science, Kobe University, Kobe

June 2018: *Developments of explicitly spin-projected electronic structure theories*, Institution for Molecular Science, Okazaki (Japanese)

June 2018: *Recent progress on the development of spin-projected methods into the weakly correlated regime*, Low-scaling and Unconventional Electronic Structure Techniques Conference (LUEST) 2018, Telluride, Colorado

August 2017: *Correlated electronic structure methods based on spin-projection for radical systems*, the 254th ACS National Meeting, Washington, DC

November 2016: *Toward an efficient description of static electron correlation by symmetry-breaking and restoration*, Third Symposium on Electronic Structure Theory, Waseda University, Tokyo

October 2016: *Correlated wave functions from spin-projected Hartree-Fock*, EMN Meeting on Computation and Theory 2016, Las Vegas, Nevada

June 2016: *Effective multi-reference configuration interaction from spin-projected HF*, Low-scaling and Unconventional Electronic Structure Techniques Conference (LUEST) 2016, Telluride, Colorado

Feburary 2015: *Constrained Density Functional Theory and beyond*, Department of Chemistry, Boston University, Massachusetts

March 2014: *Controlling spin-contamination in unrestricted Hartree-Fock*, Department of Mechanical Engineering, Stanford University, California

November 2010: *Constrained Active Space Unrestricted Mean-Field Methods for Controlling Spin-Contamination*, Department of Chemistry and Biochemistry, Waseda University, Tokyo, Japan

---

PEER-REVIEWED PUBLICATIONS

1. **Takashi Tsuchimochi**, Yoohee Ryo, Seiichiro L. Ten-no, and Kazuki Sasasako
Improved algorithms of quantum imaginary time evolution for ground and excited states of molecular systems,
Journal of Chemical Theory and Computation, *in press* (2022).
2. **Takashi Tsuchimochi**, Masaki Taii, Taisei Nishimaki, and Seiichiro L. Ten-no
Adaptive construction of shallower quantum circuits with quantum spin projection for fermionic systems,
Physical Review Research **4**, 033100 (2022).
3. Zhujun Zhang, **Takashi Tsuchimochi**, Toshiaki Ina, Yoshitaka Kumabe, Shunsuke Muto, Koji Ohara, Hiroki Yamada, Seiichiro L. Ten-no, and Takashi Tachikawa,
Binary dopant segregation enables hematite-based heterostructures for highly efficient solar H_2O_2 synthesis,
Nature Communications **13**, 1499 (2022).
4. **Takashi Tsuchimochi**, Kaname Takaoki, Kazutaka Nishiguchi, and Seiichiro L. Ten-no,
First Principles Investigation on the Heterostructure Photocatalyst Comprising BiVO4 and Few-Layer Black Phosphorus,
Journal of Physical Chemistry C **125** 21840–21850 (2021).
5. Evgeny Epifanovsky *et al.*,
Software for the frontiers of quantum chemistry: An overview of developments in the Q-Chem 5 package,
Journal of Chemical Physics **155**, 084801 (2021).
6. **Takashi Tsuchimochi**, Kosuke Yoshimura, Yuma Shimomoto, and Seiichiro L. Ten-no
Improved Description and Efficient Implementation of Spin-Projected Perturbation Theory for Practical Applications,
Journal of Chemical Theory and Computation **17**, 3471-3482 (2021).
7. **Takashi Tsuchimochi**, Yuto Mori, and Seiichiro L. Ten-no
Spin-projection for quantum computation: A low-depth approach to strong correlation,
Physical Review Research **2**, 043142 (2020).
8. **Takashi Tsuchimochi** and Seiichiro L. Ten-no
Second-order perturbation theory with spin-symmetry projected Hartree-Fock,
Journal of Chemical Theory and Computation **15**, 6688-6702 (2019).
9. **Takashi Tsuchimochi** and Seiichiro L. Ten-no
Extending spin-symmetry projected coupled-cluster to large model spaces using an iterative null-space projection technique,
Journal of Computational Chemistry **40**, 265-278 (2019). [Special Issue: Memorial Festschrift for Keiji Morokuma]
10. **Takashi Tsuchimochi** and Seiichiro L. Ten-no
Orbital-invariant spin-extended approximate coupled-cluster for multi-reference systems,
Journal of Chemical Physics **149**, 044109 (2018).
11. Michael G. Mavros, James J. Shepherd, **Takashi Tsuchimochi**, Alexandra R. McIsaac, and Troy Van Voorhis

Computational Design Principles of Two-Center First-Row Transition Metal Oxide Oxygen Evolution Catalysts,
Journal of Physical Chemistry C **121**, 15665–15674 (2017).

12. **Takashi Tsuchimochi** and Seiichiro Ten-no
Bridging Single- and Multireference Domains for Electron Correlation: Spin-Extended Coupled Electron Pair Approximation,
Journal of Chemical Theory and Computation **13**, 1667-1681 (2017).
13. **Takashi Tsuchimochi** and Seiichiro Ten-no
General technique for analytical derivatives of post-projected Hartree-Fock,
The Journal of Chemical Physics **146**, 074104 (2017).
14. Matthew Welborn, **Takashi Tsuchimochi**, and Troy Van Voorhis,
Bootstrap embedding: An internally consistent fragment-based method,
The Journal of Chemical Physics **145**, 074102 (2016).
15. **Takashi Tsuchimochi** and Seiichiro Ten-no,
Black-box description of electron correlation with spin-extended configuration interaction model: Implementation and Assessment,
Journal of Chemical Theory and Computation **12**, 1741-1759 (2016).
16. **Takashi Tsuchimochi** and Seiichiro Ten-no,
Communication: Configuration interaction combined with spin-projection for strongly correlated molecular electronic structures,
The Journal of Chemical Physics **144**, 011101 (2016).
17. **Takashi Tsuchimochi**,
Spin-Flip Configuration Interaction Singles with Exact Spin-Projection: Theory and Applications to Strongly Correlated Systems,
The Journal of Chemical Physics **143**, 144114 (2015).
18. **Takashi Tsuchimochi***, Matthew G. Welborn*, and Troy Van Voorhis,
Density Matrix Embedding In an Antisymmetrized Geminal Power Bath,
The Journal of Chemical Physics **143**, 024107 (2015).
19. **Takashi Tsuchimochi** and Troy Van Voorhis,
Time-dependent projected Hartree-Fock,
The Journal of Chemical Physics **142**, 124103 (2015).
20. Yihan Shao *et al.*,
Advances in molecular quantum chemistry contained in the Q-Chem 4 program package,
Molecular Physics **113**, 184 (2015).
21. **Takashi Tsuchimochi** and Troy Van Voorhis,
Extended Møller-Plesset perturbation theory for dynamical and static correlations,
The Journal of Chemical Physics **141**, 164117 (2014).
22. Michael G. Mavros, **Takashi Tsuchimochi**, Tim Kowalczyk, Alexandra McIsaac, Lee-Ping Wang, and Troy Van Voorhis,
What Can Density Functional Theory Tell Us about Artificial Catalytic Water Splitting?,
Inorganic Chemistry **53**, 6386 (2014).
23. Benjamin Kaduk, **Takashi Tsuchimochi**, and Troy Van Voorhis,
Analytic energy gradients for constrained DFT-configuration interaction,
The Journal of Chemical Physics **140**, 18A503 (2014).
24. Tim Kowalczyk, **Takashi Tsuchimochi**, Po-Ta Chen, Laken Top, and Troy Van Voorhis,
Excitation energies and Stokes shifts from a restricted open-shell Kohn- Sham approach,
The Journal of Chemical Physics **138**, 164101 (2013).

*These authors equally contributed to the work.

25. Carlos A. Jiménez-Hoyos, Thomas M. Henderson, **Takashi Tsuchimochi**, and Gustavo E. Scuseria,
Projected Hartree-Fock theory,
The Journal of Chemical Physics **136**, 164109 (2012).

26. Jason K. Ellis, Carlos A. Jiménez-Hoyos, Thomas M. Henderson, **Takashi Tsuchimochi**, and Gustavo E. Scuseria,
Constrained-pairing mean-field theory. V. Triplet pairing formalism,
The Journal of Chemical Physics **135**, 034112 (2011).

27. **Takashi Tsuchimochi** and Gustavo E. Scuseria,
Constrained active space unrestricted mean-field methods for controlling spin contamination,
The Journal of Chemical Physics **134** 064101 (2011).

28. **Takashi Tsuchimochi** and Gustavo E. Scuseria,
Communication: ROHF theory made simple,
The Journal of Chemical Physics **133** 141102 (2010).

29. **Takashi Tsuchimochi**, Thomas M. Henderson, Gustavo E. Scuseria, and Andreas Savin,
Constrained-pairing mean-field theory. IV. Inclusion of corresponding pair constraints and connection to unrestricted Hartree-Fock theory,
The Journal of Chemical Physics **133** 134108 (2010).

30. **Takashi Tsuchimochi**, Gustavo E. Scuseria, and Andreas Savin,
Constrained-pairing mean-field theory. III. Inclusion of density functional exchange and correlation effects via alternative densities,
The Journal of Chemical Physics **132** 024111 (2010).

31. Gustavo E. Scuseria and **Takashi Tsuchimochi**,
Constrained-pairing mean-field theory. II. Exact treatment of dissociations to nondegenerate orbitals,
The Journal of Chemical Physics **131** 164119 (2009).

32. **Takashi Tsuchimochi** and Gustavo E. Scuseria,
Strong correlations via constrained-pairing mean-field theory,
The Journal of Chemical Physics **131** 121102 (2009).

33. Alexander Thompson, Saumitra Saha, Feng Wang, **Takashi Tsuchimochi**, Ayako Nakata, Yutaka Imamura, and Hiromi Nakai,
Density functional study on core ionization spectra of cytidine and its fragments,
Bulletin of the Chemical Society of Japan **82** 187 (2009).

34. **Takashi Tsuchimochi**, Masato Kobayashi, Ayako Nakata, Yutaka Imamura, and Hiromi Nakai,
Application of the Sakurai-Sugiura projection method to core-excited-state calculation by time-dependent density functional theory,
Journal of Computational Chemistry **29**, 2311 (2008).

Reviews

1. **Takashi Tsuchimochi**,
Systematic Approach to Electron Correlation via Spin-symmetry Breaking and Restoration (Japanese),
Molecular Science **14** A0109 (2020).

Manuscripts under review or in preparation:

1. **Takashi Tsuchimochi**, Yoohee Ryo, and Seiichiro L. Ten-no
Multi-state quantum simulations via model-space quantum imaginary time evolution, arXiv:2206.04494 (2022).