Curriculum Vitae

Toshifumi Mori

Associate Professor

Institute for Materials Chemistry and Engineering, Kyushu University

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Japan

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Education:

March 2010 Ph.D. in Chemistry, Department of Chemistry, Graduate School of Science, Kyoto University, Japan

Thesis: "Theoretical Study of Dynamic Electron Correlation Effect on the Free Energy Surfaces for Chemical Reactions in Solution"

Graduate Advisor: Shigeki Kato

March 2007 Master of Science, Department of Chemistry, Graduate School of Science, Kyoto University, Japan

Thesis: "Analytical RISM-MP2 free energy gradient method and applications to organometallic compounds"

Graduate Advisor: Shigeki Kato

March 2005 Bachelor of Science, Department of Chemistry, Kyoto University, Japan

Employment:

October 2020 - present Associate Professor

Institute for Materials Chemistry and Engineering, Kyushu University

& Interdisciplinary Graduate School of Engineering Sciences, Kyushu University

April 2014 - September 2020 Assistant Professor

Department of Structural Molecular Science

The Graduate School for Advanced Studies (SOKENDAI)

December 2013 - September 2020 Assistant Professor

Department of Theoretical and Computational Molecular Science (Saito Group)

Institute for Molecular Science

Focus: Chemical reactions in protein environments and its coupling to functions, Heterogeneity in conformational dynamics of proteins

Research Experience:

April 2013 - November 2013 JSPS Postdoctoral Fellow for Research Abroad

October 2012 - November 2013 Postdoctoral Research

Department of Chemistry, University of Wisconsin, Madison Advisor: Qiang Cui

Focus: Nanoparticle - protein interactions, Protein allostery, Photochemistry under protein environments

April 2010 - September 2012 Postdoctoral Research

Department of Chemistry, Stanford University Advisor: Todd J. Martínez

Focus: Excited state dynamics in gas phase and in solution with improved ab initio electronic structure methods, Development of analytical MS-CASPT2 nonadiabatic coupling

April 2008 - March 2010 JSPS Research Fellow (DC2)

Department of Chemistry, Kyoto University

Focus: Study of organometallic reactions in solution, Developing methods to study photochemical reactions in gas phase and in solution by MS-CASPT2 method

September 2007 - March 2008 Research Assistant

Department of Chemistry, Kyoto University Advisor: Shigeki Kato

Focus: Developing methods to study organometallic reactions in solution and its applications to molecular systems

April 2005 - March 2010 Graduate Research

Department of Chemistry, Kyoto University Advisor: Shigeki Kato

Honors, Awards and Fellowships:

September 2018	Young Scientist Award, Japan Society for Molecular Science
September 2017	Early Carrier Presentation Award, The 55th Annual Meeting of The Biophysical Society of Japan
April 2013 - Nov 2013	Japan Society for the Promotion of Science (JSPS) Postdoctoral Fellowship for Research Abroad
June 2012	Poster Award, 14th International Congress of Quantum Chemistry
September 2011	Presentation Award, Annual Meeting of Japan Society for Molecular Science
April 2008 - March 2010	JSPS Research Fellowships for Young Scientist (DC2)

September 2008 Poster Award, 2008 World Congress of World Association of Theoretical and Computational Chemists (WATOC2008)

Grants:

Apr. 2018 - Mar. 2021

Grant-in-Aid for Scientific Research (C)

Apr. 2016 - Mar. 2018

Grant-in-Aid for Scientific Research on Innovative Areas (Proposed Research)

Apr. 2015 - Mar. 2018

Grant-in-Aid for Young Scientists (B)

Aug. 2014 - Mar. 2015

Grant-in-Aid for Research Activity Startup

Apr. 2008 - Mar. 2010

Grant-in-Aid for JSPS Fellows

Publications: (* co-corresponding author)

22. Y. Mori, K. Okazaki*, **T. Mori***, K. Kim*, N. Matsubayashi*, “Learning reaction coordinates via cross-entropy minimization: Application to alanine dipeptide”, *J. Chem. Phys.* **153**, 054115 (2020)

21. **T. Mori***, S. Saito*, “Dissecting the dynamics during enzyme catalysis: A case study of Pin1 peptidyl-prolyl isomerase”, *J. Chem. Theory Comput.* **10**, 3396-3407 (2020)

20. **T. Mori***, S. Saito*, "Conformational Excitation and Nonequilibrium Transition Facilitate Enzymatic Reactions: Application to Pin1 Peptidyl-Prolyl Isomerase", *J. Phys. Chem. Lett.* **10**, 474-480 (2019) *Suppl. Cover*

19. W. J. Glover, **T. Mori**, M. Schuurman, A. Boguslavskiy, O. Schalk, A. Stolow, T. J. Martínez*, "Excited state non-adiabatic dynamics of the smallest polyene, trans 1,3-butadiene. II. Ab initio multiple spawning simulations", *J. Chem. Phys.* **148**, 164303 (2018) *Featured Article*

18. A. Boguslavskiy, O. Schalk, N. Gador, W. J. Glover, **T. Mori**, T. Schultz, M. Schuurman, T. J. Martínez, A. Stolow*, "Excited state non-adiabatic dynamics of the smallest polyene, trans 1,3-butadiene. I. Time-resolved photoelectron-photoion coincidence spectroscopy", *J. Chem. Phys.* **148**, 164302 (2018) *Featured Article*

17. P. Pongprayoon*, **T. Mori***, “Critical role of dimer formation in monosaccharide binding to human serum albumin”, *Phys. Chem. Chem. Phys.* **20**, 3249-3257 (2018)

16. M. Kalathingal, T. Sumikama, **T. Mori**, S. Oiki, S. Saito*, "Structure and dynamics of solvent molecules inside Polytheonamide B channel in different environments: A molecular dynamics study", *Phys. Chem. Chem. Phys.* **20**, 3334-3348 (2018)

15. **T. Mori***, S. Saito*, "Molecular Mechanism Behind the Fast Folding/Unfolding Transitions of Villin Headpiece Subdomain: Hierarchy and Heterogeneity", *J. Phys. Chem. B* **120**, 11683-11691 (2016)

14. S. Aono, **T. Mori**, S. Sakaki*, "3D-RISM-MP2 Approach to Hydration Structure of Pt(II) and Pd(II) Complexes: Unusual H-Ahead Mode vs Usual O-Ahead One", *J. Chem. Theory Comput.* **12**, 1189-1206 (2016)

13. J. Abe‡, T. Hiyama‡, A. Mukaiyama‡, S. Son‡, **T. Mori**‡, S. Saito, M. Osako, J. Wolanin, E. Yamashita, T. Kondo, S. Akiyama*, "Atomic-scale origins of slowness in the cyanobacterial circadian clock", *Science* 349, 312-316 (2015) ‡*contributed equally*

12. **T. Mori***, S. Saito*, "Dynamic heterogeneity in the folding/unfolding transitions of FiP35", *J. Chem. Phys.* **142**, 135101 (7 pages) (2014) *Selected as one of the "2015's most read papers" in J. Chem. Phys.*

11. P. Goyal, H.-J. Qian, S. Irle, X. Lu, D. Roston, **T. Mori**, M. Elstner, Q. Cui*, "Molecular Simulation of Water and Hydration Effects in Different Environments: Challenges and Developments for DFTB Based Models", *J. Phys. Chem. B* Feature Article, **118**, 11007-11027 (2014)

10. B. Holland, **T. Mori**, T. J. Martínez*, A. G. Suits*, "Photochemical dynamics of Ethylene Cation $C_2H_4^+$", *J. Phys. Chem. Lett.* **5**, 1467-1471 (2014)

9. **T. Mori***, R. J. Hamers, J. A. Pedersen, Q. Cui*, "Integrated Hamiltonian Sampling: A Simple and Versatile Method for Free Energy Simulations and Conformational Sampling", *J. Phys. Chem. B* **118**, 8210-8220 (2014)

8. **T. Mori**, R. J. Hamers, J. A. Pedersen, Q. Cui*, "An explicit consideration of desolvation is critical to binding free energy calculations of charged molecules at ionic surfaces", *J. Chem. Theory Comput.* **9**, 5059-5069 (2013)

7. **T. Mori** and T. J. Martínez*, "Exploring the conical intersection seam by linking discrete points in the conical intersection space", *J. Chem. Theory Comput.* **9**, 1155-1163 (2013)

6. T. Kuhlman, W. J. Glover, **T. Mori**, K. B. Møller, T. J. Martínez*, "Between Ethylene and Polyenes - The Non-adiabatic Dynamics of *cis*-dienes", *Faraday Discuss.* **157**, 193-212 (2012)

5. **T. Mori**, W. J. Glover, M. Schuurman, T. J. Martínez*, "The role of Rydberg states in the photochemical dynamics of ethylene", *J. Phys. Chem. A* **116**, 2808-2818 (2012)

4. **T. Mori***, K. Nakano and S. Kato, "Conical intersections of free energy surfaces: Effect of electron correlation on a protonated Schiff base in methanol solution", *J. Chem. Phys.* **133**, 064107 (11 pages) (2010)

3. **T. Mori** and S. Kato*, “Dynamic electron correlation effect on conical intersections in photochemical ring-opening reaction of cyclohexadiene: MS-CASPT2 study”, *Chem. Phys. Lett.* **476**, 97-100 (2009)

2. **T. Mori** and S. Kato*, “Grignard Reagents in Solution: Theoretical Study of the Equilibria and the Reaction with a Carbonyl Compound in Diethyl Ether Solvent”, *J. Chem. Phys. A* **113**, 6158-6165 (2009)

1. **T. Mori** and S. Kato*, “Analytical RISM-MP2 free energy gradient method: Application to the Schlenk equilibrium of Grignard reagent”, *Chem. Phys. Lett.* **437**, 159-163 (2007)

Invited Reviews in Japanese:

5. **T. Mori***, “酵素反応の静的・動的分子機構の解明に向けて”, アンサンブル *(Ensemble) (in press)*

4. **T. Mori***, “気相・凝縮系における反応ダイナミクスの理論研究 *(Award Accounts)*”, *Molecular Science* **13**, A0106 (2019)

3. **T. Mori***, “酵素のダイナミクスは酵素反応の理解に重要か？(Are Conformational Dynamics of Enzymes Important for Enzyme Catalysis?)”, 生物物理 *(Seibutsu Butsuri)* **59**, 271-272 (2019)

2. **T. Mori***, S. Saito*, “超長時間シミュレーションで見るタンパク質のフォールディング過程 (What We can Learn about Protein Folding from Ultra-long Molecular Dynamics Simulations) ”, 生物物理 *(Seibutsu Butsuri)* **57**, 030-032 (2017)

1. **T. Mori***, “分子の光化学反応における非断熱遷移と時間分解光電子スペクトル (Theory of nonadiabatic dynamics and time resolved photoelectron spectrum for photochemistry of molecules)”, アンサンブル *(Ensemble)* **18**, 240-243 (2016)

Invited Oral Presentations (International):

3. **T. Mori**, “Hierarchy and heterogeneity in protein folding and enzyme catalysis”, 2nd workshop on Advances in Theory and Computation of Complex Systems - Biological Systems, Nanjing, December 2018

2. **T. Mori**, “Molecular study of the interplay between chemical reactions and protein conformational changes in biomolecular systems”, KAKENHI International Symposium on “Studying the Function of Soft Molecular Systems”, Sapporo, June 2017

1. **T. Mori**, “Molecular mechanism of transition dynamics in protein folding”, IAS Focused Program on Molecular Machines of Life: Simulation Meets Experiment, Hong Kong, May 2016

Invited Oral Presentations (Domestic):

11. **T. Mori**, “気相および凝縮系における反応ダイナミクスの理論的解明 (Theoretical studies of reaction dynamics in gas and condensed phases)”, 第13回分子科学討論会, 名古屋, September 2019

10. **T. Mori**, “分子シミュレーションから見たタンパク質の構造ダイナミクスと機能発現の分子機構”, 「非共有結合系分子科学研究」ワークショップ・非共有結合系の分子科学：計測技術から探る生体分子科学の新展開, Kobe, January 2019

9. **T. Mori**, “Deciphering the heterogeneous dynamics of proteins from the analysis of millisecond-long molecular dynamics simulations”, 第55回日本生物物理学会年会 (The 55th Annual Meeting of the Biophysical Society of Japan): “Softness and functions of biological molecules under various environments” session, Kumamoto, September 2017

8. **T. Mori**, “Transition path sampling法による酵素反応の遷移ダイナミクス解析”, 「レアイベントの計算科学」研究会, Atami, August 2017

7. **T. Mori**, “タンパク質のフォールディングと酵素反応の反応ダイナミクス”, 第二回計算分子科学の若手理論研究会, Kanazawa, March 2017

6. **T. Mori**, “光化学反応の多状態励起ダイナミクスと時間分解光電子スペクトル”, 「非断熱量子動力学とその周辺」研究会, Tokyo, September 2015

5. **T. Mori**, “タンパク質のフォールディング過程の動的構造解析”, 「凝縮系の理論化学」, Okinawa, March 2015

4. **T. Mori**, “効率的な自由エネルギー計算と構造サンプリングに向けたIntegrated Hamiltonian Sampling法の開発”, 新学術領域「柔らかな分子系」第9回ワークショップ, Sendai, March 2015

3. **T. Mori**, “固液界面における分子の吸着過程の分子動力学シミュレーション”, 「自然科学における階層と全体」シンポジウム, Nagoya, February 2014

2. **T. Mori**, “光異性化反応と非断熱遷移のダイナミクス”, 「化学反応のポテンシャル面とダイナミクス」研究会, Kyoto, March 2012

1. **T. Mori**, “Understanding the photochemical dynamics from first principles: The role of Rydberg state in ethylene”, 分子科学研究所・理論計算領域オープンセミナー, Okazaki, Japan, June 2011

Services:

- Journal reviewer for the *Journal of Chemical Theory and Computations, the Journal of Physical Chemistry Letters, the Journal of Physical Chemistry,* the *Journal of Chemical Physics*, *Chemical Physics Letters, PLOS ONE, CARBON*
- *Workshop organized*
  - 新学術領域「柔らかな分子系」第24回ワークショップ「若手研究者が描く分子理論の未来」, co-organizer, September 2017
- *Outreach*
  - 生物物理若手の会夏の学校・分科会講師, “長時間シミュレーションから見るタンパク質の構造遷移と機能”, August 2018
  - 分子シミュレーション夏の学校・分科会講師, “MM分科会：タンパク質の構造変化ダイナミクスと化学反応”, September 2014
  - 出前授業（甲山中学校・３年生対象）, “シミュレーションで見る生物とタンパク質”, November 2015