Rangsiman Ketkaew

Ph.D. Student in Theoretical Chemistry
Department of Chemistry, University of Zurich
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Education

- **University of Zurich** — Zürich, Switzerland
  Ph.D. Theoretical Chemistry — *2020 - Present*
  - Strong interest in quantum chemistry, enhanced sampling, machine learning
  - Advisor: Prof. Sandra Luber
- **Thammasat University** — Pathum Thani, Thailand
  M.Sc. Physical Chemistry — *2016 - 2018*
  - Strong interest in multiscale simulation of polymeric system and development of computational technique for studying electron transfer kinetics in hybrid photocatalyst
  - Advisor: Prof. Yuthana Tantirungrotechai
- **Thammasat University** — Pathum Thani, Thailand
  B.Sc. Chemistry — *2012 - 2016*
  - Emphasis on DFT and TDDFT calculations and quantum chemistry software
  - Advisor: Prof. Yuthana Tantirungrotechai

Work Experience

- **New Equilibrium Biosciences** — Boston, USA
  Consultant — *October 2019 - June 2020*
  - AWS cloud setup and system administration
  - Computational chemistry and machine learning for force-field development
  - Drug discovery based on targeting intrinsically disordered proteins (IDPs)
  - Leader: Dr. Virginia Burger (CEO and Co-founder)

Research Experience

- **National Chiao Tung University** — Hsinchu, Taiwan
  Internship student — *2018 March - April*
  - Computational Chemistry Unit, Department of Biological Science and Technology
  - Emphasis on theoretical study in photoinduced electron transfer of Ru-Re complex
  - Advisor: Prof. Jen-Shiang K. Yu (NCTU, Taiwan)
- **National Chiao Tung University** — Hsinchu, Taiwan
  Internship student — *2015 June - August*
  - Computational Chemistry Unit, Department of Biological Science and Technology

- Emphasis on mechanistic study of epoxidation reaction catalyzed by homogeneous catalysis
- Advisor: Prof. Jen-Shiang K. Yu (NCTU, Taiwan)

- **Thammasat University** Pathum Thani, Thailand
  Research assistant *Summer 2013 - 2014*
  - The role of Cu-MOFs catalyst on epoxidation with TBHP oxidant: A DFT calculation
  - Investigation of spectroscopic properties of Piperine and its derivatives
  - Effect of functional and basis set on molecular structure
  - Supervised by Prof. Yuthana Tantirungrotechai, Prof. Jonggol Tantirungrotechai (Mahidol University, Thailand), and Dr. Wikorn Punyain (Naresuan University, Thailand)

Language and Expertise

- Languages: Thai and English
- Excellent knowledge in theoretical and computational chemistry
- Excellent skill in quantum chemistry and molecular dynamics simulations
- Good skill in parallel computing and HPC system benchmark for computer software development
- Soft skills: Creative thinking, teamwork, self-learning, communication, decision making

Programming Skill

- Operating systems: Windows, UNIX and Linux (RHEL, CentOS, Ubuntu), macOS
- Cloud services: AWS (EC2, ParallelCluster, AutoScaling), Google Cloud, Colab
- Advanced: Python, IPython, Bash, C shell, Vi/Vim, LaTeX, Machine Learning, Deep Learning
- Intermediate: C++, Fortran, TCL, OpenMP, BLAS, LAPACK,
- Beginner: Compiler, MPI, LINPACK, GPU (CUDA), JavaScript, HTML/CSS,
- Application software: Git, Microsoft/Libre Office, NotePad++, Visual Studio Code
- Graphical libraries: Tachyon Graphics, Matplotlib, Plotly, PyMol, ChemDraw

Awards & Honors

- Outstanding Oral Presentation Award, The 10th Thai Student Academic Conference, Europe . 2021
- Outstanding Poster Presentation Award, The 1st TTV, IAMS, Taiwan 2018
- Best Oral Presentation Award in Physical and Theoretical Chemistry, PACCON2018 2018
- Certificates of Attendance in Atomistic Molecular Simulation Workshop 2017
- Royal Winner Award of Thailand Computational Chemistry Challenge 2016
- Best of Oral Presentation of Project in Chemistry, Thammasat University 2016
- Best Oral Presentation Award in Special Session, PACCON2016 2016
- Outstanding Oral Presentation of Special Session, PACCON2016, Thailand 2016
- Certificates of Summer Internship, Chemistry Department, Thammasat University . . 2013 - 2014

Publications

1. **R. Ketkaew**, F. Creazzo, S. Luber. Machine learning-assisted discovery of hidden states in expanded free energy space. *J. Phys. Chem. Lett.* 2022, 13, 7, 1797–1805.
DOI: 10.1021/acs.jpclett.1c04004

2. R. Han, **R. Ketkaew***, S. Luber. A concise review on recent developments of machine learning for the prediction of vibrational spectra. *J. Phys. Chem. A* 2022, 126, 6, 801–812.
DOI: 10.1021/acs.jpca.1c10417 (*selected as journal cover*)

3. **R. Ketkaew**, F. Creazzo, S. Luber. Closer look at inverse electron demand Diels–Alder and nucleophilic addition reactions on s-Tetrazines using enhanced sampling methods. *Top Catal*, 2021.
DOI: 10.1007/s11244-021-01516-y

4. M. Schilling, **R. Ketkaew***, S. Luber. How *ab initio* molecular dynamics can change the understanding on transition metal catalysed water oxidation. *CHIMIA International Journal for Chemistry*, 2021, 75, 3, 195-201(7).
DOI: 10.2533/chimia.2021.195

5. **R. Ketkaew**, Y. Tantirungrotechai, G. Chastanet, P. Guionneau, P. Harding, M. Marchivie, and D. J. Harding. OctaDist: a tool for calculating distortion parameters in spin crossover and coordination complexes. *Dalton Trans.*, 2021, 50, 1086-1096. `https://octadist.github.io`
DOI: 10.1039/D0DT03988H

6. **R. Ketkaew** and Y. Tantirungrotechai. Dissipative Particle Dynamics Study of SWCNT Reinforced Natural Rubber Composite System: An Important Role of Self-Avoiding Model on Mechanical Properties. *Macromol. Theory Simul.*, 2018, 27, 1700093
DOI: 10.1002/mats.201700093 (*selected as journal cover*)

7. T. Boonprab, P. Harding, K. S. Murray, W. Phonsri, S. G. Telfer, A. Alka¸s, **R. Ketkaew**, Y. Tantirungrotechai, G. N. L. Jamesone, and D. J. Harding. Solvatomorphism and anion effects in predominantly low spin iron(iii) Schiff base complexes. *Dalton Trans.*, 2018, 47, 12449-12458
DOI: 10.1039/C8DT02016G

8. T. Bunchuay, **R. Ketkaew**, P. Chotmongkolsap, T. Chutimasakul, J. Kanarat, Y. Tantirungrotechai, and J. Tantirungrotechai. Microwave-assisted one-pot functionalization of metal–organic framework MIL-53(Al)-NH_2 with copper(II) complexes and its application in olefin oxidation. *Catal. Sci. Technol.*, 2017, 7, 6069-6079
DOI: 10.1039/C7CY01941F

*Co-*first-authored*

Conference Presentations

1. **R. Ketkaew**, F. Creazzo, and S. Luber. *"Theoretical insight into inverse electron-demand Diels-Alder reaction and nucleophylic reactions on s-Tetrazine"*. LightChEC Symposium 2021, EMPA, Zurich, Switzerland

2. **R. Ketkaew**, Tantirungrotechai Y, and J.-S. K. Yu *"Rate parameter for the diabatic photoinduced intramolecular electron transfer of Ru(II)-Re(I) hybrid complex"*. TTV 2016, March 22-23, 2018; IAMS, Taipei, Taiwan.

3. **R. Ketkaew**, J.-S. K. Yu, and Y. Tantirungrotechai *"Theoretical study of photoinduced intramolecular electron transfer in Ru(II)-Re(I) mixed-valence complex"*. PACCON 2018, February 7-9, 2018; Hat Yai, Songkla, Thailand.

4. Sripratumwong C, **R. Ketkaew**, and Y. Tantirungrotechai *"A computational investigation of hydroxyl proton chemical shifts in ethanol clusters: a role of explicit hydrogen bonding"*. STT42, November 30 – December 2, 2016; Bangkok, Thailand

5. **R. Ketkaew**, P. Chumponanomakun, Y. Thiangjit, and Y. Tantirungrotechai *"Dissipative particle dynamics study of SWCNT reinforced natural rubber composite system: an important role self-avoiding model on mechanical properties"*. AM 2016, November 27-30, 2016; Bangkok, Thailand.

6. **R. Ketkaew**, P. Chumponanomakun, Y. Thiangjit, and Y. Tantirungrotechai *"A computational insight on the role of CNT as reinforcement filler in filled natural rubber"*. PACCON 2016, February 9-11, 2016; BITEC, Bangna, Bangkok, Thailand.

7. **R. Ketkaew**, J. Tantirungrotechai, and Y. Tantirungrotechai *"Epoxidation of styrene and cyclohexene by TBHP xxidant: a reaction mechanism investigation using density functional theory"*. PACCON 2015, January 21-23, 2015; Amari Watergate Hotel, Bangkok, Thailand.

8. K. Punyain, **R. Ketkaew**, A. Syananondh, and Y. Tantirungrotechai *"The role of exchange-correlation functional on gas phase molecular structure: a statistical assessment"*. PACCON 2014, January 8-10, 2014; Centara Hotel and Convention Centre, Khon Kaen, Thailand.

Workshop and Training

- **Big Data and Machine Learning for Chemistry** — Laussane, Switzerland
  École polytechnique fédérale de Lausanne (EPFL) — *June 7-9, 2021*
- **The 1st TTV workshop in Theoretical Chemistry** — Taipei, Taiwan
  Institute of Atomic and Molecular Sciences, Academia Sinica — *March 22-23, 2018*
- **Training in Atomistic Simulations of Biomolecules** — Trieste, Italy
  The Abdus Salam International Cente for Theoretical Physics (ICTP) — *March 6-10, 2017*
- **COLUMBUS in China 2016** — Tianjin, China
  School of Pharmaceutical Sciences and Technology, Tianjin University — *October 10-14, 2016*
- **Workshop on Applications of Materials Characterization** — Pathum Thani, Thailand
  Thailand Science Park, NSTDA — *September 26-28, 2016*
- **Workshop on Computational Biomolecular Modeling** — Bangkok, Thailand
  Faculty of Science, Kasetsart University — *July 27, 2016*
- **Workshop on Single-Crystal X-Ray Crystallography** — Pathum Thani, Thailand
  Faculty of Science and Technology, Thammasat University — *August 6-7, 2015*
- **VASP Program Workshop** — Bangkok, Thailand
  Faculty of Science, Kasetsart University — *October 21, 2015*
- **Hsinchu Summer Course and Workshop** — Hsinchu, Taiwan
  Department of Applied Chemistry, National Chiao Tung University — *July 8-10, 2015*

Academic and Community Service

- **2022:** Volunteer tutor for Swiss Chemistry Olympiad (SwissChO)
- **2021:** President of Association of Thai Students in Switzerlandahttps://www.atss-swiss.org/)
- **2021 - Present:** Teacher assistant at Department of Chemistry, Univerisyt of Zurich.
- **2019 - 2021:** Organizer of PyCon Thailand (https://th.pycon.org/en)
- **2017 - 2018:** Teacher assistant in mathematical method for chemists
- **2016 - 2018:** Teacher assistant in physical chemistry laboratory for undergraduate degree.
- **2015 - Present:** Youtube Channel: Free Online Computational Environment and Computational Chemistry Resources (in Thai). (http://bit.ly/rangsimanyoutube)
- **2015:** Head of chemistry volunteer camp 2015 for rural development. (https://sites.google.com/site/chemactivity)
- **2014 - 2018:** Web administrator of Computational Chemistry Research Unit, Thammasat University. (https://sites.google.com/site/compchem403)
- **2012 - 2013:** Physics & chemistry tutor at Academic Student Club, Thammasat University.

References

- **Assoc. Prof. Dr. Sandra Luber**
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  Faculty of Science
  University of Zurich, CH-8057, Zurich, Switzerland
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  Website: https://www.chem.uzh.ch/en/research/groups/luber.html
- **Assoc. Prof. Dr. Yuthana Tantirungrotechai**
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  Faculty of Science and Technology
  Thammasat University, Pathum Thani, 12120 Thailand
  E-Mail: yt203y@gmail.com & yuthana_t@sci.tu.ac.th
  Website: https://sites.google.com/site/compchem403/people/faculty/yuthana
- **Prof. Dr. Jen-Shiang K. Yu**
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  Website: http://wild.life.nctu.edu.tw/~jsyu/
- **Prof. Dr. David J. Harding**
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