Rangsiman Ketkaew

Ph.D. Student in Computational Chemistry and Machine Learning
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Educations

- **University of Zurich** — Zurich, Switzerland
  Ph.D. Computational Chemistry and Machine Learning — *June 2020 - Aug 2024*
  - Interests: *Ab initio* Molecular dynamics, Enhanced sampling, Machine learning for molecular design and catalysis, Reaction network, Neural network
  - Advisor: Prof. Dr. Sandra Luber
- **Thammasat University** — Pathum Thani, Thailand
  M.Sc. Computational Chemistry — *July 2016 - December 2018*
  - Interests: Multiscale coarse-graining method, Constrained density functional theory, Intramolecular electron transfer, Hybrid photocatalysts
  - Advisor: Prof. Dr. Yuthana Tantirungrotechai
- **Thammasat University** — Pathum Thani, Thailand
  B.Sc. Chemistry — *May 2012 - June 2016*
  - Interests: Mechanistic study, Density functional theory, Excited state dynamics
  - Advisor: Prof. Dr. Yuthana Tantirungrotechai

Work Experiences

- **New Equilibrium Biosciences** — Boston, USA
  Drug Discovery Chemist and System Administrator — *October 2019 - June 2020*
  - Develop machine learning force-field targeting intrinsically disordered proteins
  - Design and setup AWS cloud-based parallel distributed cluster
  - Benchmark and fine-tune molecular dynamics software
  - Leader: Dr. Virginia M. Burger (CEO and Co-founder)
- **Thinking Machines Data Science** — Bangkok, Thailand
  Machine Learning Consultant — *August 2021 - November 2021*
  - Develop machine learning (time-series) model for predicting fouling in heat exchanger
  - Provide expert guidance and domain skills in chemistry
  - Leader: Promphorn Chaichirawiwat (Country Manager)

Research Experiences

- **National Chiao Tung University** — Hsinchu, Taiwan
  Internship student — *Summer 2015 & 2018*
  - 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

Technical Skills

- Proficient: Python, Fortran, C++, Bash, Vim, MySQL, LaTeX
- Experienced: Distributed Computing, ETL/ELT, CI/CD, System Integration, VS Code
- Familiar: BLAS, LAPACK, OpenMP, LINPACK, ScaLAPACK
- Chemistry/Biology Software: CP2K, Gaussian, NWChem, RDKit, Gromacs, Schrödinger
- ML Frameworks: TensorFlow, PyTorch, NumPy, Scikit-learn, Pandas
- Tools/Platforms: AWS (EC2, ParallelCluster and AutoScaling), Git, Docker, Kubernetes

Awards & Honors

- CMSZH Travel Award, University of Zurich, Switzerland 2024
- Best Oral Presentation, CMSZH Retreat 2022, Switzerland 2022
- Outstanding Poster Presentation Award, The 1st TTV, IAMS, Taiwan 2018
- Best Oral Presentation Award in Physical and Theoretical Chemistry, PACCON 2018 2018
- Certificates of Attendance in Atomistic Molecular Simulation Workshop 2017
- Royal Winner Award of Thailand Computational Chemistry Challenge 2016
- Best Senior Project, Department of Chemistry, Thammasat University 2016
- Best Oral Presentation Award in Special Session, PACCON 2016 2016

Selected Publications

Peer-Reviewed Articles

1. **R. Ketkaew**, F. Creazzo, K. Sivula and S. Luber. A Metadynamics Study of Water Oxidation Reactions at (001)-WO_3/liquid-water Interface. *Accepted to publish in Chem Catalysis*
2. **R. Ketkaew** and S. Luber. DeepCV: A Deep Learning Framework for Blind Search of Collective Variables in Expanded Configurational Space. *J. Chem. Inf. Model. 2022, 62, 24, 6352-6364.* (https://lubergroup.pages.uzh.ch/deepcv)

3. F. Creazzo, **R. Ketkaew**, K. Sivula, S. Luber. Effects of surface wettability on (001)-WO_3 and (100)-WSe_2: A spin-polarized DFT-MD study. *Appl. Surf. Sci.* 2022, 601, 154203.

4. **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.

5. 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. (*featured on the journal cover*)

6. **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, 65, 1-17.

7. M. Schilling, **R. Ketkaew***, S. Luber. How *ab initio* molecular dynamics can change the understanding on transition metal catalysed water oxidation. *CHIMIA*, 2021, 75, 3, 195-201(7).

8. **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`)

9. **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 (*featured on the journal cover*)

Books

1. **R. Ketkaew**. Machine Learning for Quantum Chemistry 2022 (in Thai)

2. **R. Ketkaew**. Algorithms for Computer Simulation of Molecular Systems 2023 (in Thai)

**Co-first-authored*

Conference and Workshop

- **Machine Learning of First Principles Observables** — Berlin, Germany
  CECAM-DE-MMS — *July 8-12, 2024*
- **59th Symposium on Theoretical Chemistry** — Zurich, Switzerland
  ETH Zurich — *September 11-14, 2023*
- **58th Symposium on Theoretical Chemistry** — Heidelberg, Germany
  University of Heidelberg — *September 18-22, 2022*
- **20 years of Metadynamics** — Laussane, Switzerland
  CECAM-HQ-EPFL — *June 5-8, 2021*
- **Chasing CVs using Machine Learning** — Paris, France
  Inria and CECAM-FR-MOSER — *June 28-30, 2022*
- **Big Data and Machine Learning for Chemistry** — Laussane, Switzerland
  École polytechnique fédérale de Lausanne (EPFL) — *June 7-9, 2021*

Academic and Community Service

- **2022 - 2023:** Core Team Member of Google Developer Student Club ETH Zurich (https://gdsc.community.dev/eth-zurich)
- **2022 - 2024:** Tutor for Swiss Chemistry Olympiad (SwissChO)
- **2021:** Core organizer of Thailand Machine Learning for Chemistry Competition (https://tmlcc2021.devpost.com)
- **2021 - 2023:** Teaching assistant for "Physical Chemistry I and II" courses, Department of Chemistry, University of Zurich.
- **2021:** President of Association of Thai Students in Switzerland (https://www.atss-swiss.org)
- **2019 - 2021:** Organizer, PyCon Thailand (https://th.pycon.org/en)

References

- **Prof. Dr. Sandra Luber**
  Department of Chemistry, University of Zurich, CH-8057, Zurich, Switzerland
  E-Mail: sandra.luber@chem.uzh.ch, Website: https://www.luber-group.com
- **Dr. Fabrizio Creazzo**
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- **Prof. Dr. Yuthana Tantirungrotechai**
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  E-Mail: yt203y@gmail.com, Website: https://sites.google.com/site/compchem403
- **Prof. Dr. Jen-Shiang K. Yu**
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