Rangsiman Ketkaew | Researcher

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I am a Swiss graduate who is legally eligible to work in Switzerland (Federal Law: Art. 21 Precedence)

Professional Experience

ETH Zürich **Zurich**
Postdoctoral Machine Learning Researcher *2025–Present*
- Develop GNN-based transformer models for solvation free energies prediction and uncertainty quantification of chemical reaction networks in explicit solvent phase
- Design a scalable architecture of graph transformer for 3D molecular geometry (15% faster than the reference models)
- Create a novel transition states dataset of organic molecules at the DFT and CCSD(T) levels using ORCA software
- Implement ML workflow into SCINE software, interfacing with PyTorch Geometric for energy gradient calculations

Cloud HM **Bangkok**
Technical Writer *2021-2023*
- Wrote monthly articles about AWS cloud computing with a focus on product updates, solution architecture, use cases in basic research, and healthcare science.

New Equilibrium Biosciences **Boston, MA**
Machine Learning Scientist for Drug Discovery *2020*
- Developed ML force field for drug discovery targeting intrinsically disordered proteins (IDPs)
- Optimized long-range interaction calculation in GROMACS software with 10% better performance

Cloud Architect *2019*
- Designed AutoScaling Parallel Cluster with GPUs on AWS cloud for high-performance calculations
- Optimized AWS cloud workflows to maximize cost-efficiency and reduce operational expenses (20% cost saving)

Thinking Machines Data Science **Bangkok**
Machine Learning Consultant *2020–2020*
- Developed time-series ML model for forecasting fouling in heat exchangers
- Provided expert guidance and domain skills in chemical engineering processes
- Curated high-quality dataset of chemical compounds with heuristic features using quantum chemistry aspect

Education

University of Zurich **Zurich**
PhD in Machine Learning and Computational Chemistry *2020 - 2025*
- Thesis: Development of collective variables using electronic structure and statistical techniques
- DeepCV: An automated autoencoder with MLOps for molecular structure search (Project lead)

NCTU **Taiwan**
Internship *2016 & 2018*
- Symmetry-adapted cluster/configuration interaction (SAC-CI) for chemical reaction mechanism investigation

Thammasat University **Bangkok**
BSc & MSc in Physical Chemistry *2012 - 2018*
- Thesis: Dissipative particle dynamics simulation of mechanical properties of composite nano-materials
- OctaDist: A tool for calculating distortion parameters of metal complexes (Project lead)
- High-throughput DFT and semiempirical (DFTB) and spectrum calculations for catalyst and reaction mechanism design

Side Projects

mlff: Information about many aspects of foundational ML quantum chemistry models (e.g. UMA and MACE)

QM-Perf: Scaling benchmarking of quantum chemistry software (ORCA, NWChem, Q-Chem, PySCF, Gaussian, Turbomole) on a shared-memory parallel cluster

MoleView: A fast and lightweight webapp plug-in for 3D molecular visualization

Technical Skills

Programming Languages

Python: Develop deep learning models for scientific applications and sparse matrix multiplication on a GPU-distributed cluster (libraries: PyTorch, TensorFlow, JAX)

Fortran: Interface CP2K with TensorFlow C++ for training ML energy and gradient.

C++: Implemented collective variables in PLUMED and implemented transformer-based ML models in SCINE

Quantum Chemistry and Molecular Simulation Tools

Software: CP2K (developer), NWChem (contributor), ORCA, PySCF, TBlite/xTB, ASE, Turbomole

Toolkit: DeepCV (developer), PLUMED (contributor), RDKit, OpenMM, OpenForceField, DeePMD-kit

Software Development Experience

MLOps/DevOps: Built a scaling ML workflow on ETH Euler cluster and tested with GitLab CI/CD pipeline

Data warehouse: Designed a backend for large-scale chemical datasets using Snowflake, MongoDB and Databricks

AWS: Designed parallel computing workflow using ParallelCluster, AutoScaling and Lustre file system

CUDA: Integrated CuPy into PLUMED (a library for enhanced sampling simulation) for real-time model training

MPI: Improved parallel strategy of metadynamics simulation code in CP2K software

Publications

Selected Peer-Reviewed Articles

2026: **R. Ketkaew**, S. Jog, G.-G. Gosálbez and S. Luber. Symbolic Regression Collective Variables for Enhanced Sampling Simulations *(reviewed)*

2024: D. Tang, **R. Ketkaew**, and S. Luber. Machine learning interatomic potentials for heterogeneous catalysis *Chemistry–A European Journal* 30 (60), e202401148

2022: **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

2022: 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*)

Books (in English and Thai)

2023: **R. Ketkaew** Algorithms for Computer Simulation of Molecular Systems (Link)

2022: **R. Ketkaew** Machine Learning for Quantum Chemistry (Link)

Awards and Honors

2024: CMSZH Travel Award, University of Zurich — Switzerland

2018: NCTU Elite Scholarship, NCTU — Taiwan

2017: Visiting Scholarship, ICTP, Trieste — Italy

2016: Royal Winner Award of Thailand Computational Chemistry Challenge — Thailand

Volunteer and Community Service

2022 - 2023: Core team member of Google Developer Student Club ETH Zurich (Link)

2022 - 2024: Tutor for Swiss Chemistry Olympiad (SwissChO), ETH Zurich/UZH

2021: Lead organizer of Thailand Machine Learning for Chemistry Competition (Link)

2021 - 2023: Teaching assistant for Physical Chemistry I and II, Department of Chemistry, UZH

2019 - 2021: Organizer, PyCon Thailand