

Rangsiman Ketkaew



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EXPERIENCES

COMPUTATIONAL CHEMISTRY GROUP | DOCTORAL STUDENT

June 2020 – August 2024 | Zurich, Switzerland

- Develop techniques in quantum chemistry, machine learning, and statistical techniques for free energy calculation, molecular design and chemical reaction
- Build automatic deep learning workflow with MLOps/DevOps strategies

NEW EQUILIBRIUM BIOSCIENCES | COMPUTATIONAL CHEMIST AND SYSTEM ADMINISTRATOR

October 2019 – June 2020 | Boston, USA

- Design and setup AWS cloud-based autoscaling parallel cluster with GPUs for high-performance calculations
- Develop machine learning force field for drug discovery targeting intrinsically disordered proteins (IDPs)

THINKING MACHINES DATA SCIENCE | MACHINE LEARNING CONSULTANT

August 2021 - November 2021 | Bangkok, Thailand

- Develop machine learning model for predicting fouling in heat exchangers
- Provide expert guidance and domain skills in chemistry

PROJECTS

CP2K & PLUMED | FORTRAN & C++

2020 - Present

- Implement electronic-based collective variables using density functional perturbation theory for metadynamics enhanced sampling methods

DAENN/DEEPCV | PYTHON & C++

2021 - Present

- Neural network framework and library interfacing with TensorFlow for automatic learning collective variables for metadynamics simulations

OCTADIST | PYTHON

2019 - 2020

- Project leader of the OctaDist – a computer framework for calculating distortion parameters of transition metal complexes

CONTRIBUTIONS

2023	Google Developer Student Club ETH Zurich	Core Team Member
2021	Thailand Machine Learning Competition	Lead Organizer
2020-2023	HackZurich	Participant
2019	Kaggle's Predicting Molecular Properties	Participant

AWARDS

2024	CMSZH Travel Award Machine learning workshop	Berlin, Germany
2022	CMSZH Best Oral Presentation	Savognin, Switzerland
2018	NCTU Elite Internship Program	Hsinchu, Taiwan
2017	Visiting Scholarship at ICTP	Trieste, Italy
2016	The Winner of Computational Chemistry Challenge	Bangkok, Thailand

SKILLS

PROGRAMMING

Proficient:

Python • Fortran • C++ • Bash • Vim • MySQL • L^AT_EX

Experienced:

Distributed Computing • ETL/ELT • CI/CD • System Integration

Familiar:

OpenMP • OpenMPI • LINPACK • BLAS • LAPACK

LIBRARIES/Frameworks

TensorFlow • PyTorch • NumPy • Scikit-learn • Pandas • VS Code

TOOLS/Platforms

AWS • Git • Docker • Kubernetes

EDUCATIONS

UNIVERSITY OF ZURICH

PH.D. IN COMPUTATIONAL CHEMISTRY AND MACHINE LEARNING

June 2020 - September 2024 | Zurich,

Switzerland

Department of Chemistry

THAMMASAT UNIVERSITY

MASTER'S IN COMPUTATIONAL CHEMISTRY

December 2018 | Pathum Thani, Thailand

Department of Chemistry

THAMMASAT UNIVERSITY

BACHELOR'S IN CHEMISTRY

June 2016 | Pathum Thani, Thailand

Department of Chemistry

REFERENCES

Sandra Luber, Professor in Theoretical Chemistry, University of Zurich, Switzerland

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Virginia M. Burger, CEO and Co-founder, New Equilibrium Biosciences, Boston, USA

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