

Rajdeep (Ron) Sarma

✉ rsarma@andrew.cmu.edu [ronsarma.github.io/](https://github.com/ronsarma) [ronsarma](https://github.com/ronsarma) [in rajdeep-sarma](https://www.linkedin.com/in/rajdeep-sarma)

Education

- PhD Carnegie Mellon University**, Chemistry Pittsburgh, USA
Aug 2022 – Present
- Principal Investigator: Dr Isaac Garcia-Bosch (GPA: 3.61/4.0) ([IGB Lab](#))
 - Topics: Physical Chemistry, Catalysis, Machine Learning
- BS-MS Indian Institute of Science Education and Research Bhopal**, Chemistry Bhopal, India
Aug 2016 – May 2021
- Masters' Supervisor: Dr Debasish Manna (GPA: 7.85/10.0) ([DM Lab](#))
 - Topics: Chemical Biology, DNA (De)methylation, Inorganic Chemistry

Experience

- Research Assistant**, Team lead - Project [EQUUS](#) Aug 2024 – Present
- Supervisors: Dr Isaac Garcia-Bosch and Dr Olexandr Isayev
 - Lead a team of 7, developed a [workflow](#) for ultrafast theoretical screening of >800k organic molecules
 - Tools used: [*Computational*] Python, PyTorch, RDKit, JavaScript, HTML, CSS, SQL, DFT (ω B97M-D3BJ/Def2-TZVPP), MLIP/NNP (AIMNet2). [*Experimental*] $^1\text{H-NMR}$, Cyclic Voltammetry and Automated Experimentation
- Research Assistant**, Electron-Coupled Proton Buffers (ECPBs) Jan 2023 – Aug 2024
- Supervisor: Dr Isaac Garcia-Bosch
 - Experimental study of the thermochemistry of a new class of molecular systems: $6\text{H}^+/6\text{e}^-$ and $4\text{H}^+/4\text{e}^-$ ECPBs
 - Tools used: [*Synthetic*] Organic and Inorganic Synthesis, Workups, Crystallizations, Glove-Box Techniques. [*Analytical*] $^1\text{H-NMR}$, CV, Open-Circuit Potential, UV-vis Spectroscopy, Mössbauer and X-Ray Diffraction
- Teaching Assistant** Aug 2022 - Dec 2023
- Course mentorship: 30 students (over 3 semesters). Research mentorship: 8 students (over varying durations)
- Conferences**
- NVIDIA GTC 2025: Training and networking Washington DC, Oct 2025
 - RE+ 2025: [NSF I-corps Regional](#) funded visit for customer discovery Las Vegas, Sept 2025
 - ACS Fall 2025: Poster presentation on the updated Project EQUUS v1.1.0 Washington DC, Aug 2025
 - ACS Spring 2025: Two talks ($6\text{H}^+/6\text{e}^-$ ECPBs and the initial Project EQUUS v1.0.0) San Diego, March 2025

Publications

Machine Learning-Accelerated Screening of Hydroquinone Analogs for Proton-Coupled Electron Transfer

ChemRxiv, Nov 2025, doi: [10.26434/chemrxiv-2025-9k7p7](https://doi.org/10.26434/chemrxiv-2025-9k7p7)

Sarma, R., Wang, Y., Hebert, D., Tran, E., Shao, C., Fu, S., Cho, I., Isayev, O., Garcia-Bosch, I.

Stepwise $6\text{H}^+/6\text{e}^-$ Electron-Coupled-Proton Buffers based on Fe and Redox-Active Ligands

ACS Inorg. Chem., Sept 2025, doi: [10.1021/acs.inorgchem.5c02720](https://doi.org/10.1021/acs.inorgchem.5c02720)

Sarma, R., Wu, T., Ye, D., Qiu, Y. L., Park, S., Cohen, E., Xiong, J., Guo, Y., Garcia-Bosch, I.

Tuning the Thermochemistry and Reactivity of a Series of Cu-Based $4\text{H}^+/4\text{e}^-$ Electron-Coupled-Proton Buffers

ACS Inorg. Chem., 2024, doi: [10.1021/acs.inorgchem.4c00835](https://doi.org/10.1021/acs.inorgchem.4c00835)

Wu, T., Puri, A., Qiu, Y. L., Ye, D., **Sarma, R.**, Wang, Y., Kowalewski, T., Siegler, M., Stewart, M., Garcia-Bosch, I.

A Chemical Model of a TET Enzyme for Selective Oxidation of Hydroxymethyl Cytosine to Formyl Cytosine

ACS Inorg. Chem., 2023, doi: [10.1021/acs.inorgchem.3c00063](https://doi.org/10.1021/acs.inorgchem.3c00063)

Patil, D., Kundu, S., Pain, P. K., **Sarma, R.**, Manna, D.

Courses

Introduction to Deep Learning - 11785 (Fall 25)

[Course Website](#)[Course Project](#)

- Instructors: Dr Bhiskha Raj and Dr Rita Singh
- Tools Used: Python (OOP, NumPy, SciPy), PyTorch (data handling and preprocessing, optimizers, schedulers), Cloud Computing (AWS, GCP, Kaggle, Colab), WandB, Various Network Architectures (RNN, CNN, VAE, etc)

Algorithms for Big Data - 15851 (Spring 25)

[Course Website](#)[Course Project](#)

- Instructor: Dr David P Woodruff
- Tools Used: Linear Algebra, Multivariable Calculus, Probability Theory, Computational Complexity Theory, Sketching, Information Theory, Advanced ML techniques (clustering based data-efficient training and HyperAttention)

Introduction to Machine Learning - 10701 (Fall 24)

[Course Website](#)[Course Project](#)

- Instructors: Dr Geoffrey J Gordon and Dr Maria-Florin Balcan
- Tools Used: Python (OOP, NumPy, SciPy, Scikit-learn, PyTorch), Active Learning, Reinforcement Learning, Information Theory, VC dimensions, Rademacher Complexity, Clustering, Boosting, Various Model Architectures

Neural Networks and Deep Learning in Science - 09616 (Spring 24)

- Instructor: Dr Olexandr Isayev
- Tools Used: Python (OOP, NumPy, Pandas, SciPy, Scikit-learn, PyTorch), Classification, Regression, Clustering, Boosting, Classic NN Architectures (ResNet, LeNet, AlexNet, VGG, CNN, RNN, etc)

Computational Modeling, Statistical Analysis and Machine Learning in Science - 09615 (Fall 22)

- Instructor: Dr Olexandr Isayev
- Tools Used: Python (NumPy, Pandas, SciPy, Scikit-learn), Statistics (bias, variance, overfitting, regularization), Exploratory Data Analysis (elbow method, dimensionality reduction, outlier detection)

Awards

Samuel S Wang Travel Award

Nov 2025

An annual [departmental travel grant](#) awarded to an individual for covering expenses during conference visits.

NSF I-Corps Regional

Aug 2025 - Sept 2025

This is an [NSF funded program](#) designed to train academics to convert university spin-off technologies into start-ups.

INSPIRE Fellowship

Aug 2016 - May 2021

The Innovation in Science Pursuit for Inspired Research ([INSPIRE](#)) fellowship is awarded by the Government of India.

Skills

Programming Languages:

Python, Bash, Git, HTML, CSS, JavaScript

Technical stack:

[*Data Science*] NumPy, Pandas, SciPy, Scikit-learn, dimensionality reduction methods (PCA, tSNE, UMAP)

[*Machine Learning*] PyTorch and associated cuda-x libraries for processing audio/video/molecular inputs

[*Cloud Computing*] Amazon Web Services (AWS), Google Cloud Platform (GCP), Kaggle, Weights and Biases (WandB)

[*Computational Chemistry*] RDKit, ASE, Machine Learned Interatomic Potentials (MLIP), Density Functional Theory (DFT)

Chemistry:

[*Synthetic*] Organic and inorganic synthesis, chromatographic purification techniques, air and moisture sensitive techniques (Schlenk line and glove box), distillation and crystallization (vapor diffusion and layering)

[*Analytical*] 1D and 2D NMR, cyclic voltammetry, open-circuit potential, UV-vis spectroscopy, Mössbauer, x-ray diffraction, elemental analysis, mass spectrometry (electron-spray ionization and gas chromatography), infrared spectroscopy