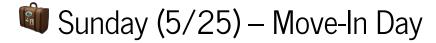


# Welcome to the SIMCODES REU Bootcamp

May 25-30, 2025

• Free donuts and science await!



- Move-In: 9 AM 5 PM at Freddy Court
- Alternative arrangements: contact PI/Co-PI
- Tip: Pack light, bring curiosity



8:50 AM - 3 PM

Mentors: Ryan, Felix

Icebreakers & donuts

- What is SIMCODES?
- Safety, integrity, and expectations
- Fundamentals of Reactions



- Types of chemical reactions
- Endo vs exothermic
- Kinetics: 🕲 + 🤚 + 🧪
- Reaction mechanisms & equilibrium



## Tuesday – Setup Day

### Mentor: Ryan

- AMES & ISU ID cards 🗎
- Software Development Environment (SDE)
  - Linux terminal
  - Python installation
  - Run code from terminal
- Lunch at Union Drive
- Git & GitHub: version control crash course



### Why version control?

- Git basics: commit, push, pull
- Cookiecutter for repo setup



## Mednesday – Research + Engineering

Mentors: Davit, Myra

- Bootcamp Overview
- Enzymes as Catalysts (Part 1)
- Intro to Software Engineering

Note: Lunch on your own today



## Thursday – Al & Quantum Day

Mentors: Qi, Mengdi, Peng

- Intro to Machine Learning (Parts 1 & 2)
- Hands-on ML with Colab: scikit-learn, pytorch, matplotlib
- Quantum Chemistry with Peng / 8



- Run models on Colab
- Evaluate & visualize performance

Friday – Molecular Dynamics + Wrap-Up

Mentors: Davit & Xueyu

- What is Molecular Dynamics?
- How we simulate molecules in motion
- Cool fact: atoms never sleep 😌



• Time: TBD 📢 🕡

Hosted by all mentors

A great time to relax, bond, and nerd out \( \operatorname{\operatorname{o}} \)



## Modeling Serine Protease Catalysis

Exploring Enzyme Mechanisms in Synthetic Micelle Environments

### Mentors: Xueyu Song, Davit Potoyan

- Investigate how serine proteases function within synthetic micelle environments.
- Utilize molecular dynamics simulations to model substrate interactions.
- Gain insights into enzyme catalysis mechanisms in non-traditional settings.

Serine Protease Model

REU intro 5/30/25, 12:46 PM



## Automating Protein Fragmentation

Streamlining Protein Analysis through Automation

Mentors: Qi Li, Ryan Richard, Theresa Windus

- Develop algorithms to automate the fragmentation of complex proteins.
- Enhance computational efficiency in protein structure analysis.
- Apply methods to facilitate large-scale protein modeling tasks.

Protein Fragmentation



## ML-Enhanced Modeling of Metal-Protein Interactions

Integrating Machine Learning with Computational Chemistry

Mentors: Peng Xu, Mark Gordon, Qi Li, Mengdi Huai

- Employ machine learning techniques to predict metal-binding sites in proteins.
- Combine quantum chemistry calculations with data-driven models.
- Advance understanding of metalloprotein functions and interactions.

Metal-Protein Interaction



- 💢 A Glimpse into Cutting-Edge Research
  - Modeling Serine Protease Catalysis: Delving into enzyme mechanisms within synthetic environments.
  - Automating Protein Fragmentation: Revolutionizing protein analysis through automation.
  - ML-Enhanced Metal-Protein Modeling: Merging machine learning with computational chemistry for advanced insights.

BootCamp Projects





- Molecular Dynamics Simulations: GROMACS, NAMD
- Quantum Chemistry Software: Gaussian, ORCA
- Machine Learning Frameworks: TensorFlow, PyTorch
- **Programming Languages:** Python, C++, R

### Research Tools

!-- slide -->



- Enzymes are biological catalysts that speed up reactions.
- They achieve this by lowering the activation energy of a chemical reaction.
- Key idea: Enzymes stabilize the transition state.

#### Overall reaction:

$$S \stackrel{E}{\longrightarrow} P$$

REU\_intro



## Energy Landscape of a Catalyzed Reaction

## Energy Diagram

- **Uncatalyzed**: high activation energy.
- Catalyzed: enzyme stabilizes the transition state, lowering the energy barrier.



- Substrate binds at the enzyme's active site.
- Two models of binding:
  - Lock and Key: perfect fit.
  - Induced Fit: enzyme changes shape upon binding.

### **Binding pathway:**

$$1.E + S \rightleftharpoons ES$$

2. 
$$ES 
ightarrow E + P$$



### Michaelis-Menten Kinetics

#### Reaction mechanism:

$$E+S{\overset{k_1}{
ightleftharpoons}}ES{\overset{k_{ ext{cat}}}{\longrightarrow}}E+P$$

Michaelis-Menten rate law:

$$v = rac{V_{ ext{max}}[S]}{K_M + [S]}$$

Where:

- $V_{
  m max} = k_{
  m cat} [E]_{
  m total}$
- ullet  $K_M=rac{k_{-1}+ar{k}_{
  m cat}}{k_{1}}$



## ✓ Typical Michaelis—Menten Curve

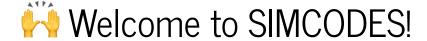
### Michaelis-Menten curve

### Michaelis-Menten curve

- As [S] increases, v approaches  $V_{\mathrm{max}}$ .
- $K_M$  is the [S] at which  $v=rac{V_{ ext{max}}}{2}$ .



- Enzymes speed up reactions by lowering activation energy.
- Binding involves specific interactions and sometimes conformational change.
- Michaelis-Menten kinetics models how reaction velocity depends on [S].



We're excited to have you.

Let's code, simulate, and discover together \*\*\*

Slides: github.com/SIMCODES-ISU/training\_materials

Questions? Ask your mentors or throw them into the Slack!

## Time for some Python tutorials!

https://dpotoyan.github.io/Statmech4ChemBio/

Speaker notes