🧬 Welcome to the SIMCODES REU Bootcamp

May 25–30, 2025

- Free donuts and science await!

🧳 Sunday (5/25) – Move-In Day

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

👋 Monday – Orientation + Chemistry Kickoff

8:50 AM – 3 PM

Mentors: Ryan, Felix

- Icebreakers & donuts 🍩
- What is SIMCODES?
- Safety, integrity, and expectations
- Fundamentals of Reactions

🔥 Reactions & Thermochemistry (Monday PM)

- 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

🔃 Git & GitHub (Tuesday PM)

Why version control?

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

🔬 Wednesday – Research + Engineering

Mentors: Davit, Myra

- Bootcamp Overview 🧭
- Enzymes as Catalysts 🪩 (Part 1)
- Intro to Software Engineering 👩‍💻

Note: Lunch on your own today

🤖 Thursday – AI & 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 🧪⚛️

🧪 ML Practice Goals (Thursday PM)

- 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 😴

🎉 Friday Night: Boardgames & Pizza!

- Time: TBD 🍕🎲
- Hosted by all mentors
- A great time to relax, bond, and nerd out 😄

🧬 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.

🤖 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.

🤖 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.

🎓 REU BootCamp Project Showcase

🌟 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.

🛠️ Tools & Technologies

🧰 Empowering Research with Advanced Tools

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

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🧬 What is Enzyme Catalysis?

- 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:

$$S \xrightarrow{E} P$$

Energy Landscape of a Catalyzed Reaction

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

🔗 Enzyme–Substrate Binding

- 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. $ES \rightarrow E + P$

Michaelis–Menten Kinetics

Reaction mechanism:

$$E + S \underset{k_{-1}}{\overset{k_1}{\rightleftharpoons}} ES \xrightarrow{k_{\text{cat}}} E + P$$

Michaelis–Menten rate law:

$$v = \frac{V_{\max}[S]}{K_M + [S]}$$

Where:

- $V_{\max} = k_{\text{cat}}[E]_{\text{total}}$
- $K_M = \frac{k_{-1} + k_{\text{cat}}}{k_1}$

Typical Michaelis–Menten Curve

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

🧠 Summary

- 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].

🙌 Welcome to SIMCODES!

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