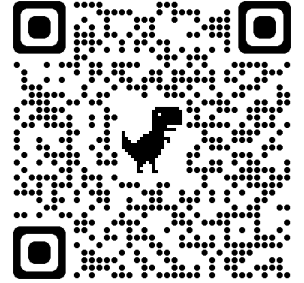# Mentor Introductions

SIMCODES 2025
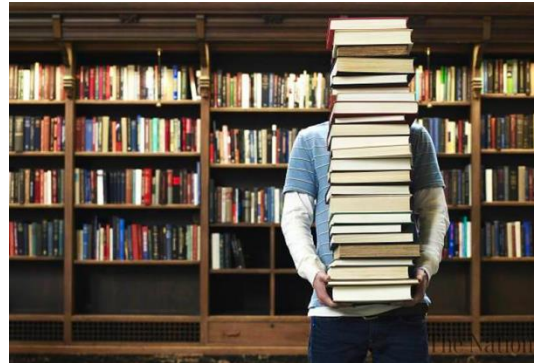
Qi Li

- My name
  - Name can tell a lot
  - Gender, Ethnicity, Age, Religion, …
  - Important feature for many NLP tasks
- My background
  - BS. Math
  - MS. Stats
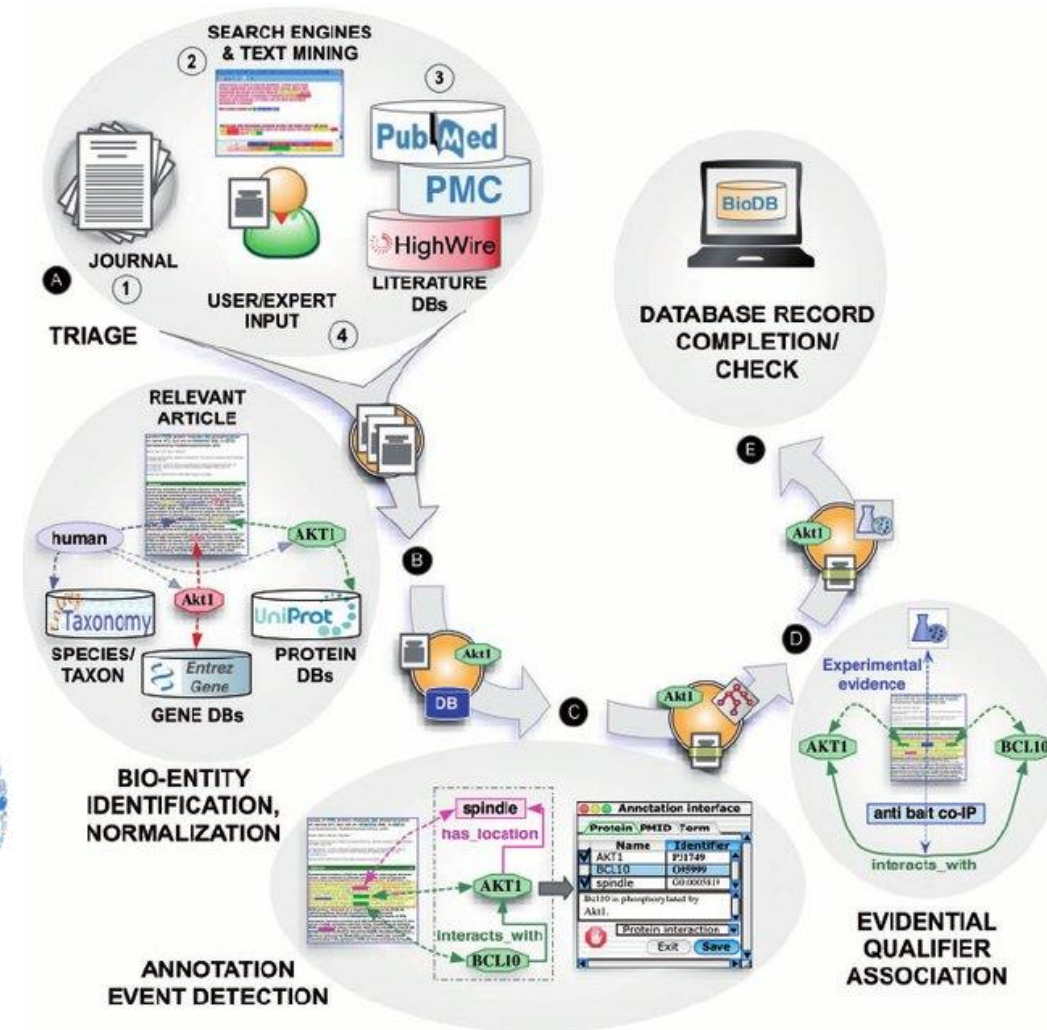 - PhD. CS

My research

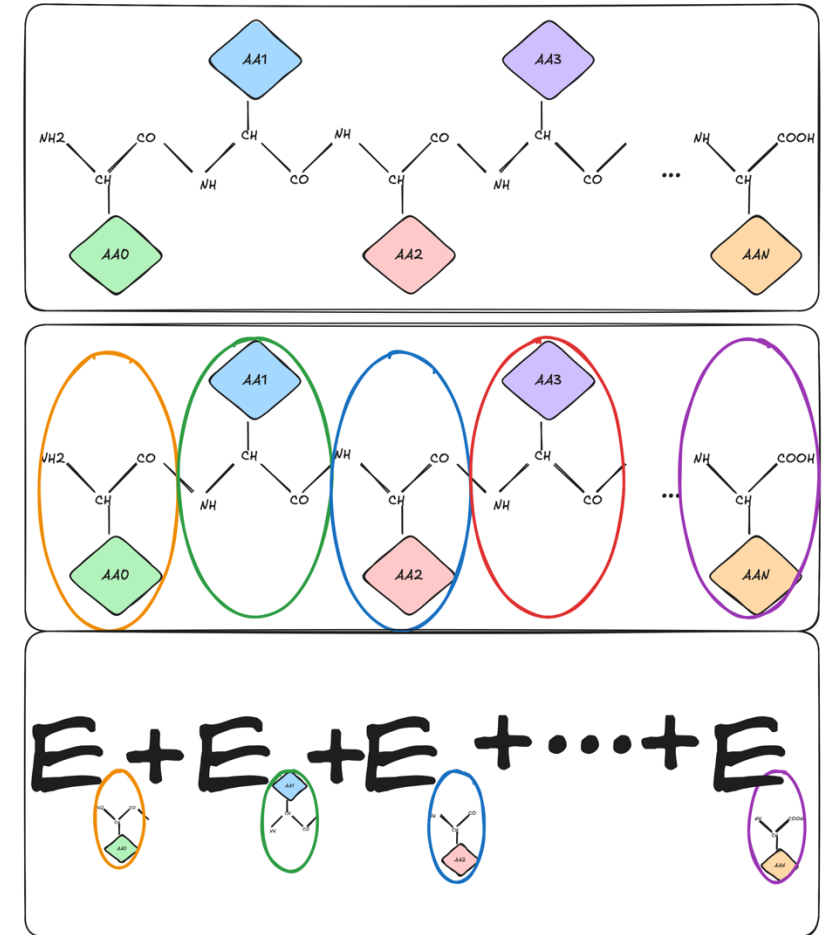- NLP -- Information extraction
- Generation models
- Applied ML

Knowledge & Insights

SIMCODES Project:
Developing components for automating fragmentation

- Mentee: Gabriela and Devarsh

- Goals:
  - Function for identifying amino acids in a protein.
  - Function for splitting a protein by amino acid.
  - Idea: protein as an unnatural language
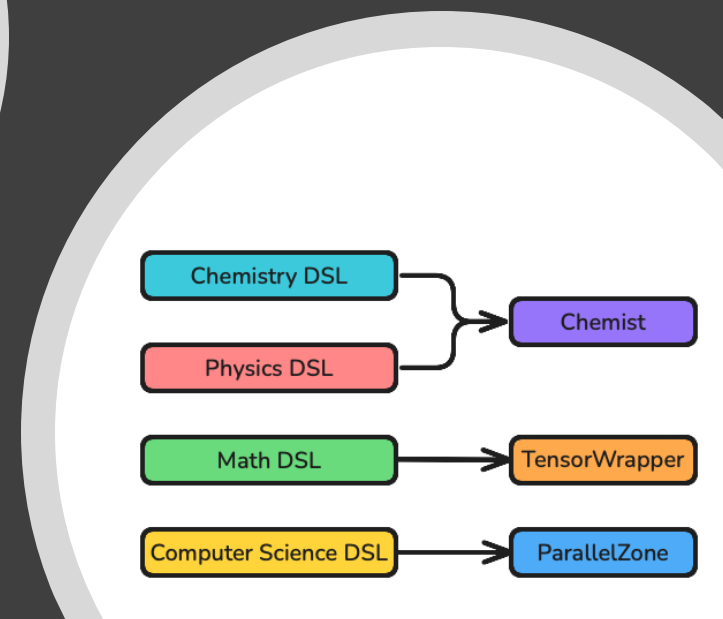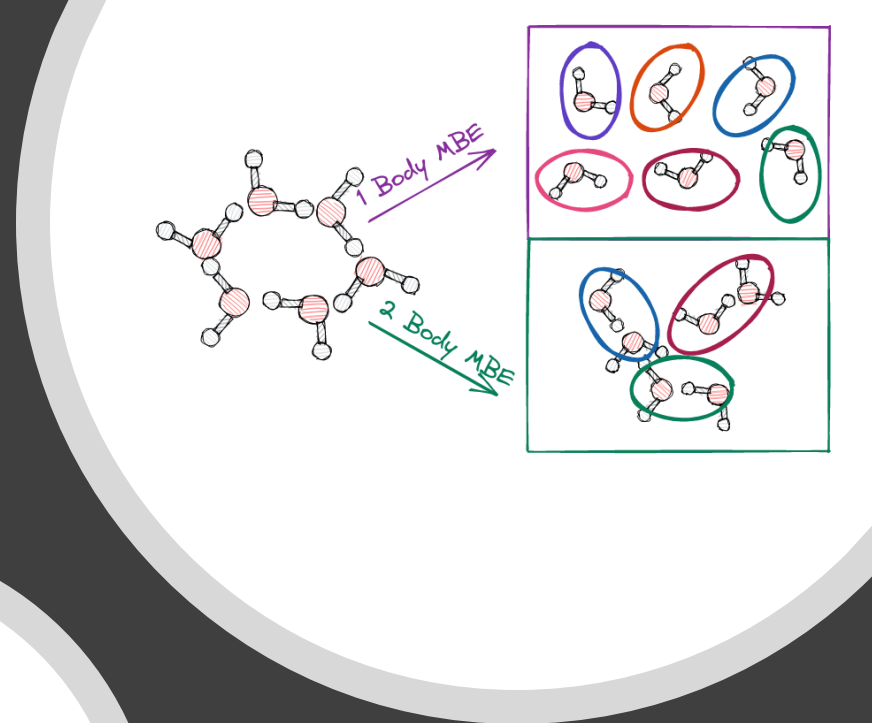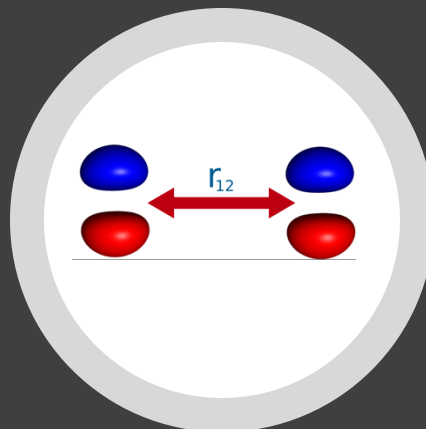
Computer Science

Ryan Richard

- Scientist at Ames National Laboratory and Adjunct Professor of Chemistry at Iowa State University.

- Background: Grew up in Ohio, PhD in chemistry from "The" Ohio State University.

- Interests: travel, technology, video games, exercise, being told what to do by my dogs.
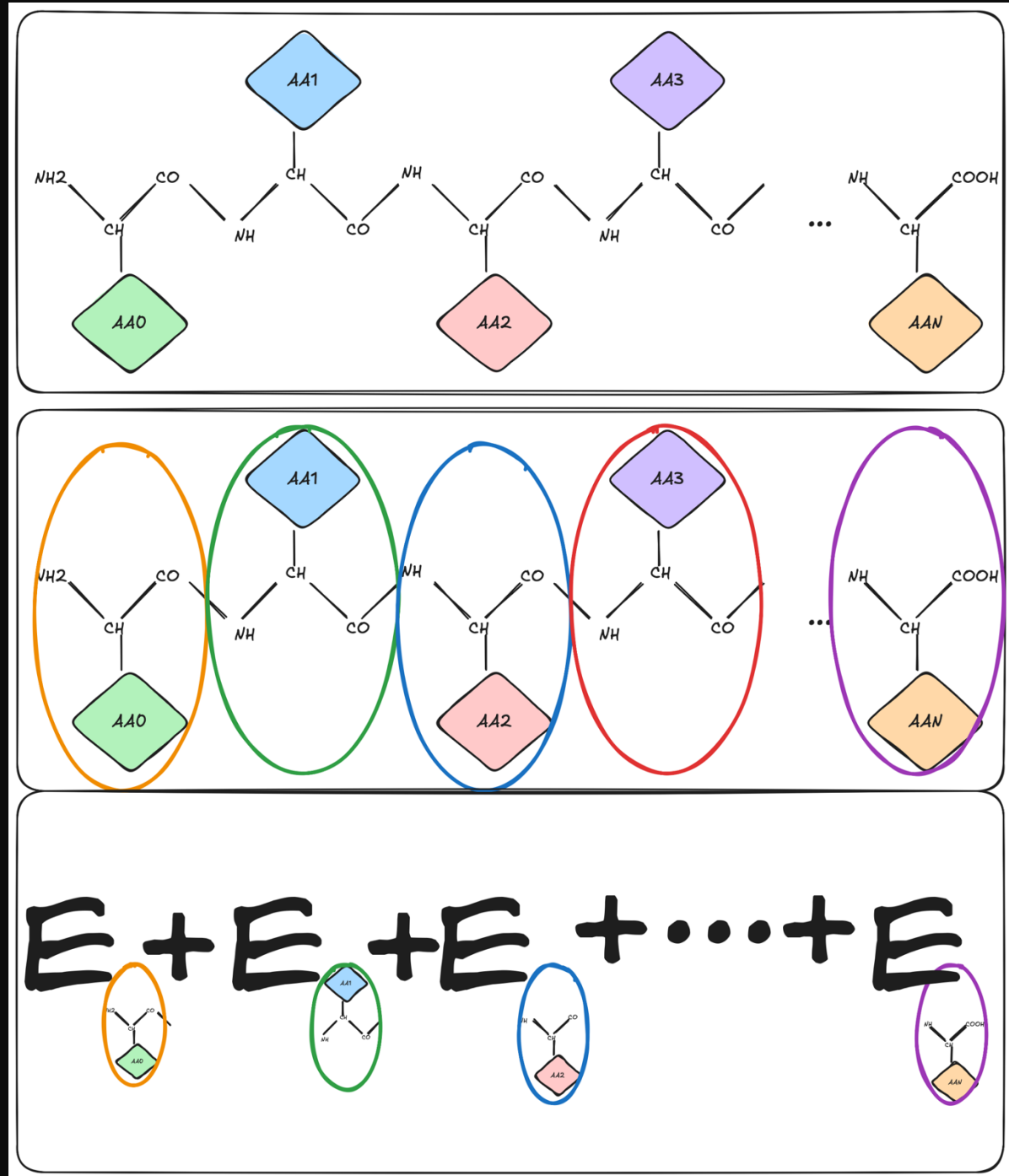
Research in the Richard Group

- Research interests: Sustainable scientific software development, high-performance computing, reduced scaling electronic structure theory.

- Develop for NWChemEx ecosystem.

- Strong emphasis on software engineering applied to theoretical chemistry.

SIMCODES Project: Developing components for automating fragmentation

- Mentee: Daniel Woodard

- Summary: Winner-take-all battle between Daniel's chemical intuition and the best AI/ML model Gabriela and Devarsh can make.

- Goals:
    - Develop tools for reading PDF files.
    - Function for identifying amino acids in a protein.
    - Function for splitting a protein by amino acid.

The Richard and Windus Groups