Mentor Introductions

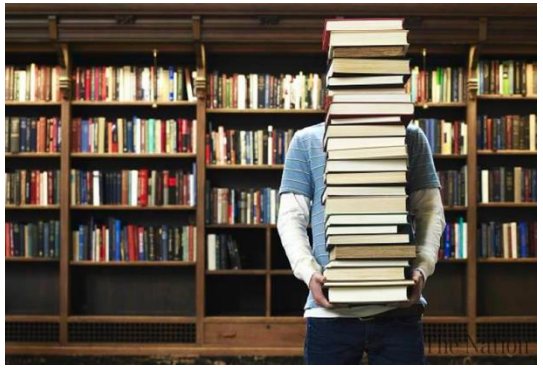
SIMCODES 2025

Qi Li

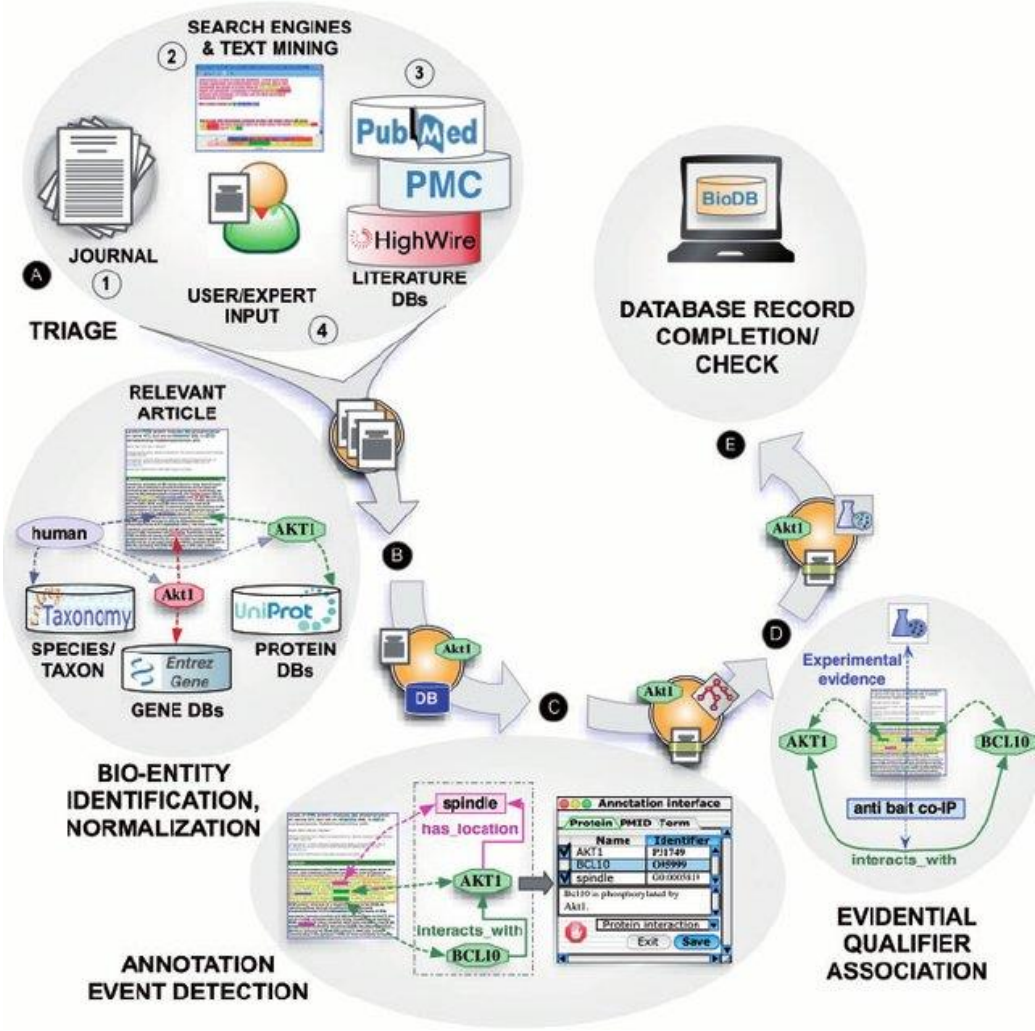
- My name
  - Name can tell a lot
  - Gender, Ethnicity, Age, Religion, …
  - Important feature for many NLP tasks
- My background
  - BS. Math
  - MS. Stats
  - PhD. CS

My research

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

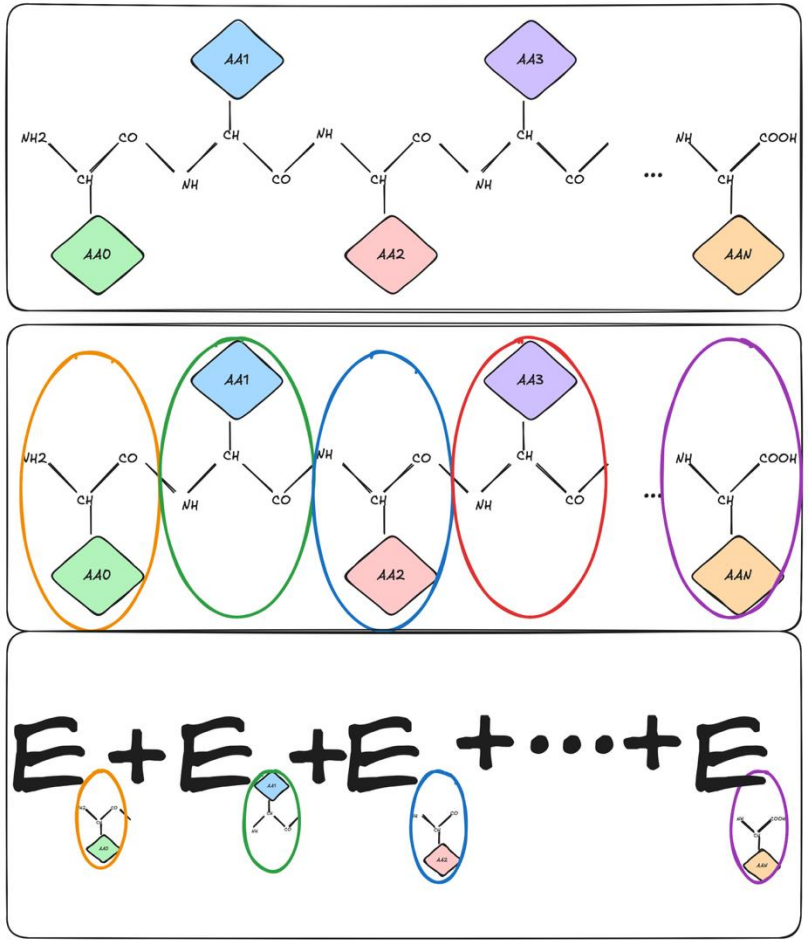


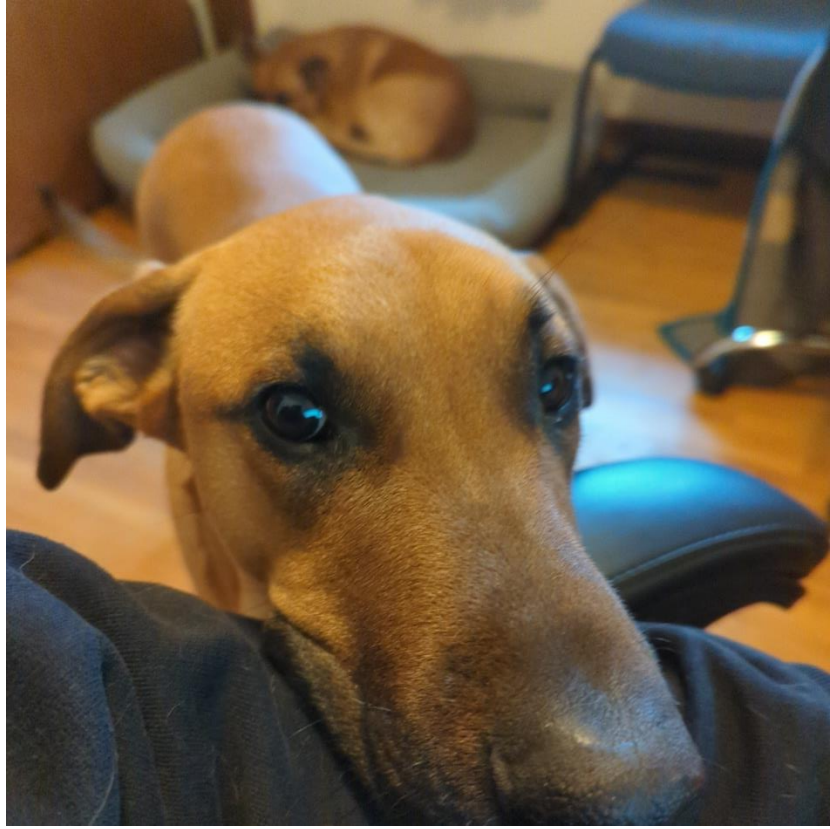
Knowledge
& Insights



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



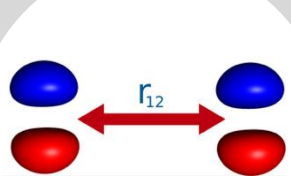


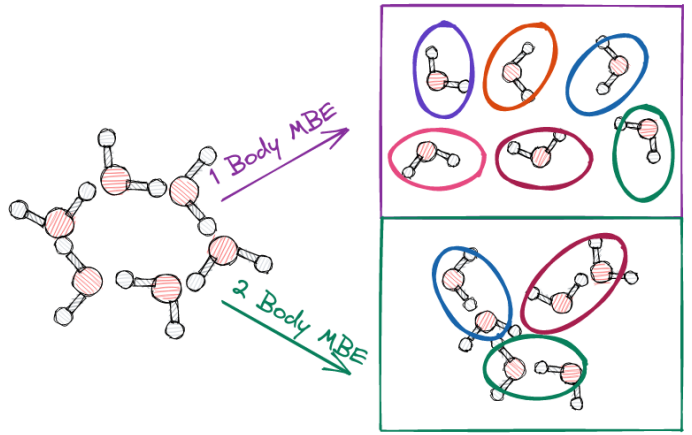
Ryan Richard

- 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.

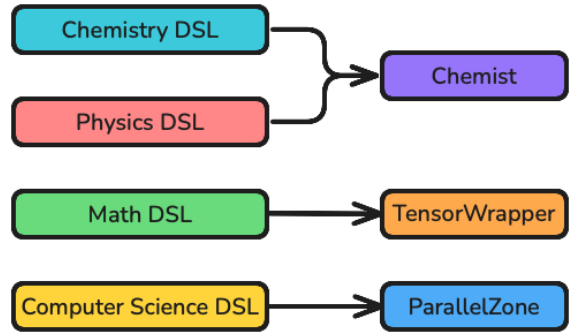




PluginPlay

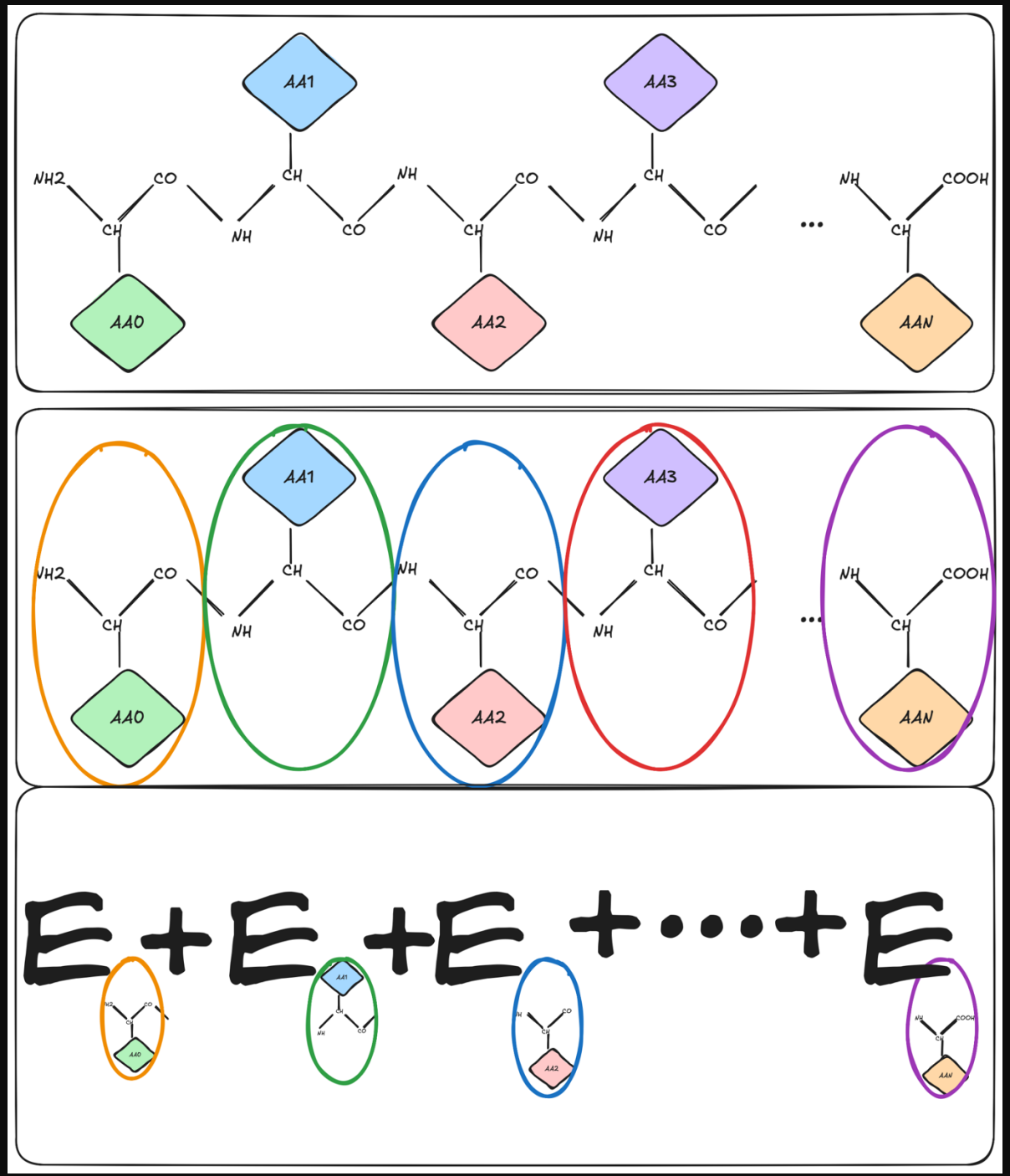
NWChemEx

SimDE



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

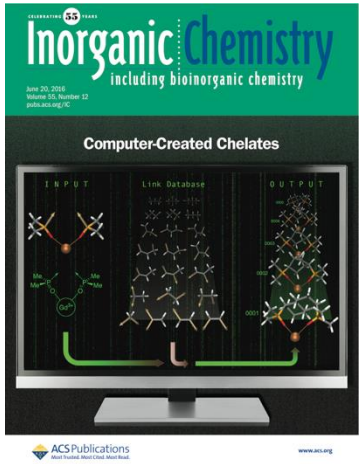
Research in Song's Group

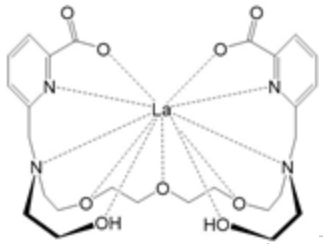
Statistical Mechanics and Biophysics at Iowa State University

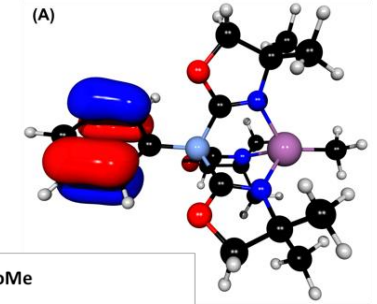
- Electron Transfer and Energy Transfer in Photosynthesis and Electric Cells, electron transport in DNA
- Solvation Dynamics and Dielectric Fluctuations in Inhomogeneous Dielectric Materials, such as Protein and Nucleic Acids
- Theory of Protein Crystallization and protein-protein interaction
- Molecular Debye-Huckel theory of ionic fluids
- Phase behaviors and nucleation
- Sub-diffraction imaging using heterodyne and entangled photons
- Studies of nano-domains of supercooled liquids using machine learning

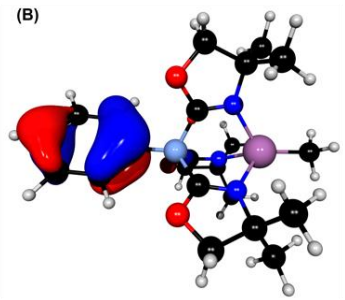
The Windus Group

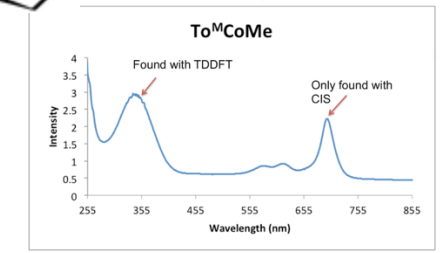
Separations and catalysis challenges



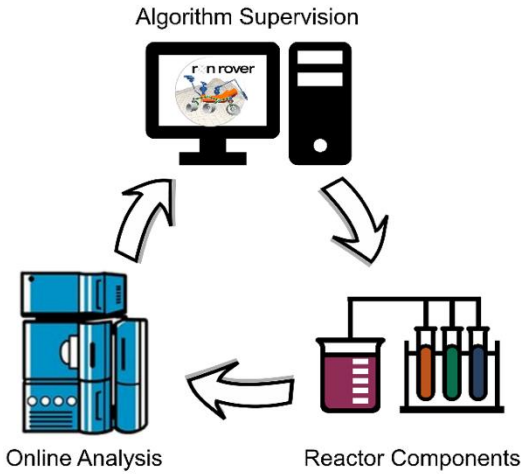




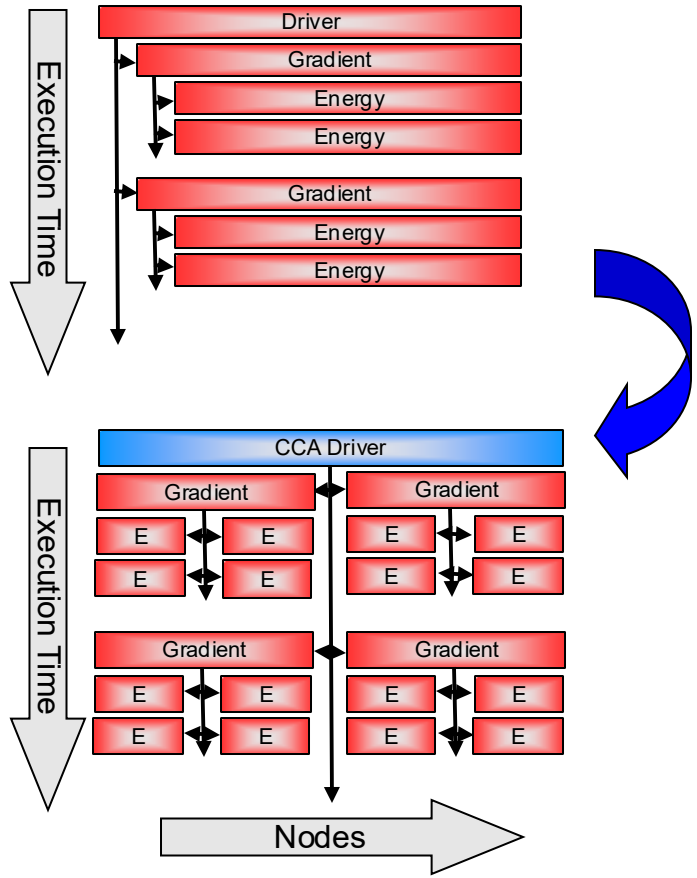




Reaction optimization and lab automation



High performance, exascale computing



The Windus Group and Funding

rxn rover

CMI Accelerating Energy Innovations

NWChemEx

DEPARTMENT OF ENERGY · UNITED STATES OF AMERICA

AIR FORCE OFFICE OF SCIENTIFIC RESEARCH · UNITED STATES AIR FORCE

NSF

AMES NATIONAL LABORATORY 1947 75 2022

MolSSI

- Scientist II, Ames National Laboratory
- Adjunct assistant professor, Department of Chemistry
- pxu@iastate.edu
- pxu@ameslab.gov

- What is your area of research?
  - Theoretical and Computational Chemistry
  - developer of General Atomic and Molecular Electronic Structure System (GAMESS) package
  - Reduced scaling electronic structure theory
  - Heterogeneous high-performance computing and energy efficient computing
- Research Interests
  - Protein-ligand interactions; drug design
  - Heterogeneous catalysis modeling
  - Radical chemistry
  - Quantum computing and machine learning
- How do you relax at the end of the day?
  - Play with my kid; play games