CHEM 4(6)PB3

pip install chemistry

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@RoVargasHdz

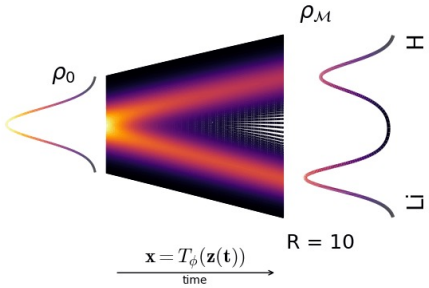
Who am I?

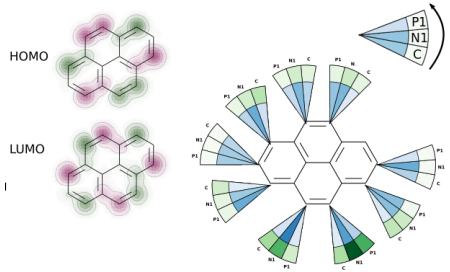
- Born in Mexico city
- Undergraduate: UNAM
  - comp. chemistry
- PhD: UBC Vancouver, BC
  - ML/AI for Chemistry
- Postdocs: UofT
  - more ML/AI and Chemistry
- Hobbies: cycling and coffee

not me

ChemAI group

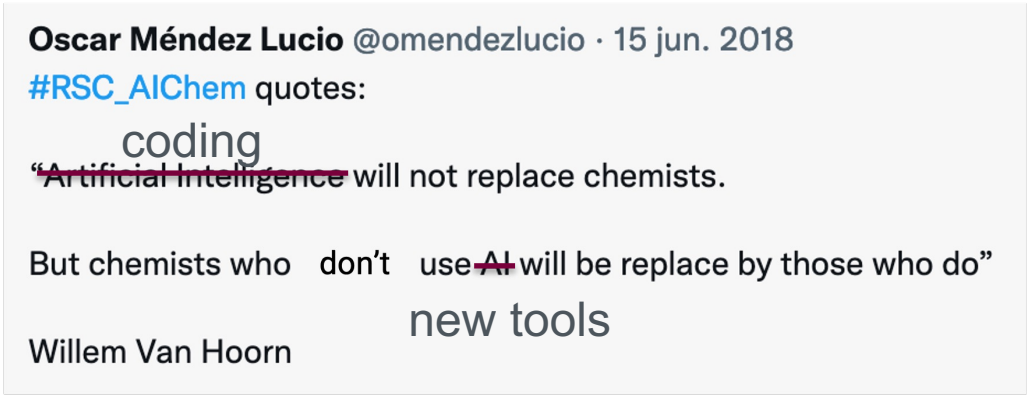
- more** ML/AI and Chemistry/Physics
- new comp. tools for simulating chemistry
- Chem 4PB3 (chemoinf. + python + ML)





Goal

Do NOT be afraid of coding!



Evaluation

Course component		Marks	Notes
Assignment 0 **Deadline: Jan 24th**		0%	Warm up
(midterm) Assignment 1 **Deadline: Feb 28th**		**20%**	(Haven't designed yet) Load a data set. Basic data analysis Some simple model fitting
Final project **Deadline: Final exam**	Oral presentation	20%	25 min: 15 + 5 + 5
	Code	25%	Code (Google Colab)
	Written report	25%	Maximum 6 pages, without refs. single column
	Total	**75%**	
Democracy	**10%**		Feedback from the group and myself

* If you decide no to hand Assignment 1, do a super Final project.

There is no homework so there isn't an excuse for not spending time on your final project

Outline

- Introduction to programming in Python
  numpy, pandas, matplotlib, scipy
- Recap of calculus and linear algebra
  linear regression and gradient descent
- Chemoinformatics
  RDKit, PyMOL, …
- Computational Chemistry*
  Hartree-Fock and Density Functional Theory

*the depth will depend on how we advance in the course

Final Project

Examples:

1. Published paper: Reproduce part of a work.
2. Lab project: Automating data analysis
3. Model fitting
4. Comp. Chem.: Simulation of a series of compounds
    1. Potential energy surface for a chem. rxn
    2. Transition state search

Undergraduates
team <= 2
Graduate students
team = 1

Final Report

Section I: Introduction, literature review and problem statement (1.5 pages)

Section II: Hypothesis (0.5 pages)

Section III: Describe the model/data or chemical system (1 page)

Section IV: Results (2.5 pages)

Section V: Summary (1 page)

Section V: Future work (0.5 pages)

Section VIII: References (not included in the page limit)

Final Presentation

Time limit:

Total 25 minutes:

15-20 min: present your work

5-7 min: go-through a working demo using your (part) code

5 min: questions (part of your mark!)

Colab demo:

Google Colab demo that was used in your final project

(example) **https://github.com/RodrigoAVargasHdz/steady_state_jax**

VA

What are the most relevant skills for a computational chemistry now a days?

In computational chemistry, some of the most relevant skills include:

1. Familiarity with quantum chemistry methods: These methods are used to model the electronic structure of molecules and predict their properties.
2. Experience with molecular modeling software: These programs are used to build and analyze chemical systems.
3. Programming skills: Many computational chemistry tasks involve automating tasks or analyzing large datasets, so being able to program can be very useful.
4. Knowledge of statistical analysis: This can be helpful for analyzing and interpreting the results of computational chemistry simulations.
5. Familiarity with drug design: Many computational chemists work on developing new drugs, so understanding the principles of drug design can be important.
6. Good communication skills: Computational chemistry often involves collaborating with researchers from other disciplines, so being able to clearly communicate your work is important.

VA What are the most relevant topics for a modern computational chemistry course?

Here are some topics that might be covered in a modern computational chemistry course:

1. Quantum chemistry methods: This could include topics such as Hartree-Fock theory, density functional theory, and wavefunction-based methods.
2. Molecular mechanics: This includes classical methods for modeling the behavior of molecules, such as molecular dynamics and Monte Carlo simulations.
3. Molecular dynamics simulations: This involves using computational methods to model the movement of atoms and molecules over time.
4. Drug design: This could include topics such as virtual screening, docking, and pharmacophore modeling.
5. Materials modeling: This could include topics such as predicting the properties of solid materials or modeling the behavior of surfaces.
6. Statistical analysis: This could include topics such as hypothesis testing, regression analysis, and machine learning.
7. High-performance computing: This could include topics such as parallel computing and optimization for running simulations on supercomputers.
8. Data analysis: This could include topics such as visualizing and interpreting the results of computational simulations.

What do you want to learn?

This course is for you!

Questions about ML/AI?

Chemistry in the Era of Artificial Intelligence

Yi Luo*

Artificial Intelligence in Chemistry: Current Trends and Future Directions

Zachary J. Baum*, Xiang Yu, Philippe Y. Ayala, Yanan Zhao, Steven P. Watkins, and Qiongqiong Zhou

How AI is Changing Chemical Discovery?

Victor Hugo Cano Gil

AI in science and life

References

Use the internet!