



CHEM-4PB3 (2023)

Chemistry + Computer Science

Who am I?

1. Born in Mexico (**I'm Millennial**)
2. Undergraduate in Theoretical Chemistry
3. PhD at UBC (Vancouver) ML + Physics (2013-2019)
4. Postdoc at UofT (2019-2022)

Goal

Do NOT be afraid of coding

Oscar Méndez Lucio @omendezlucio · 15 jun. 2018

#RSC_AIChem quotes:

“Artificial Intelligence will not replace chemists.

But chemists who don't use AI will be replaced by those who do”

Willem Van Hoorn

Evaluation

1. Final project

- i. Oral presentation → 20 to 30 min
- ii. Online tutorial → code or data set for reproducibility
- iii. Two written reports:
 - a. Midterm report (maximum 2 pages, deadline: week after reading break)
 - b. Final report (maximum 6 pages)

2. Tutorials & coding exercises

-To help you develop the skills needed for your final project

Final project

Examples,

1. Reproduce some results of a published paper
2. Data analysis for a lab project
3. Theoretical study:
 - i. potential energy surface for a reaction
 - ii. transition state search
 - iii. ...
4. Parameter fitting for model

Outline

1. Introduction to programming (**Python**)

2. Linear algebra and calculus (**refresh**)

3. **Machine learning***

i. Regression models

ii. Classification models

iii. Optimization algorithms

4. **Computational Chemistry***

i. Hartree-Fock

ii. Density Functional Theory

iii. Molecular Dynamics

Final report

1. Section 1: Introduction, literature review and problem statement (**midterm report**)
2. Section 2: Hypothesis (**midterm report**)
3. Section 3: Describe your data/model or chemical system (**midterm report**)
4. Section 4: Results
5. Section 5: Summary
6. Section 6: Future work
7. Section 8: References (not included in the page limit)

Final presentation

Time limit:

20 to 30 min included questions and a go-through the working demo.

Colab demo:

Colab demo that explains and displays the model/data used for the problem of interest.

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

Software

1. Machine Learning

- i. [Scikit learn](#)
- ii. [Jax ecosystem](#)
- iii. [PyTorch](#)

2. Data science

- i. [Numpy](#)
- ii. [Matplotlib \(or Seaborn\)](#)
- iii. [SciPy](#)
- iv. [Pandas](#)

Software

3. Computational Chemistry

i. [PySCF \(or others\)](#)

ii. [RDKit](#)

iii. Molecular Dynamics: [JaxMD](#), [TorchMD](#), [openMD](#)

iv. Visualization

What do you want to learn?

- This course is for you!



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.

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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.

