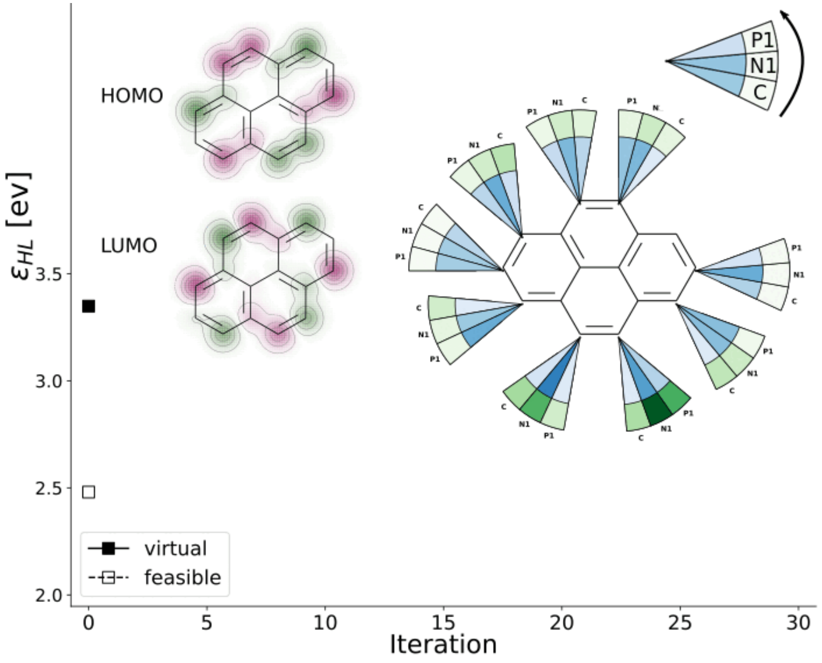

CHEM-4PB3 (2022)

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# Chemistry + Computer Science
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Goal

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Do NOT be afraid of coding
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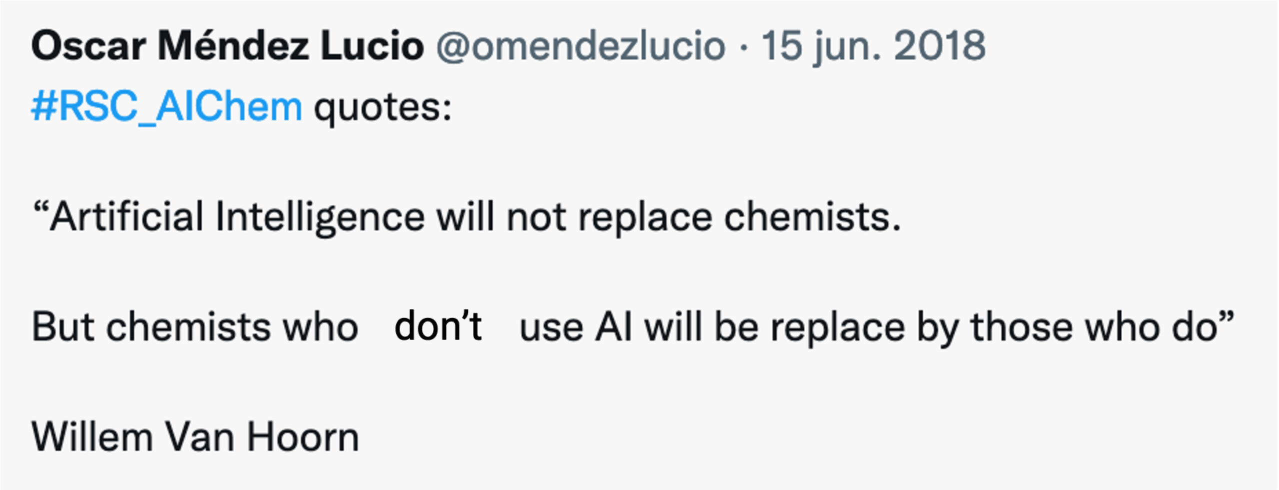


Oscar Méndez Lucio @omendezlucio · 15 jun. 2018
#RSC_AIChem quotes:

“Artificial Intelligence will not replace chemists.

But chemists who don’t use AI will be replace by those who do”

Willem Van Hoorn

Evaluation

1. **Final project**
    1. Oral presentation → 20 to 30 min
    2. Online tutorial → code or data set for reproducibility
    3. Two written reports:
        1. Midterm report (maximum 2 pages, deadline: week after reading break)
        2. 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. pontential energy urface 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***
    1. Regression models
    2. Classification models
    3. Optimization algorithms
4. **Computational Chemistry***
    1. Hartree-Fock
    2. Density Functional Theory
    3. Molecular Dynamics

Tentative topics

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)

4 to 6 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)**

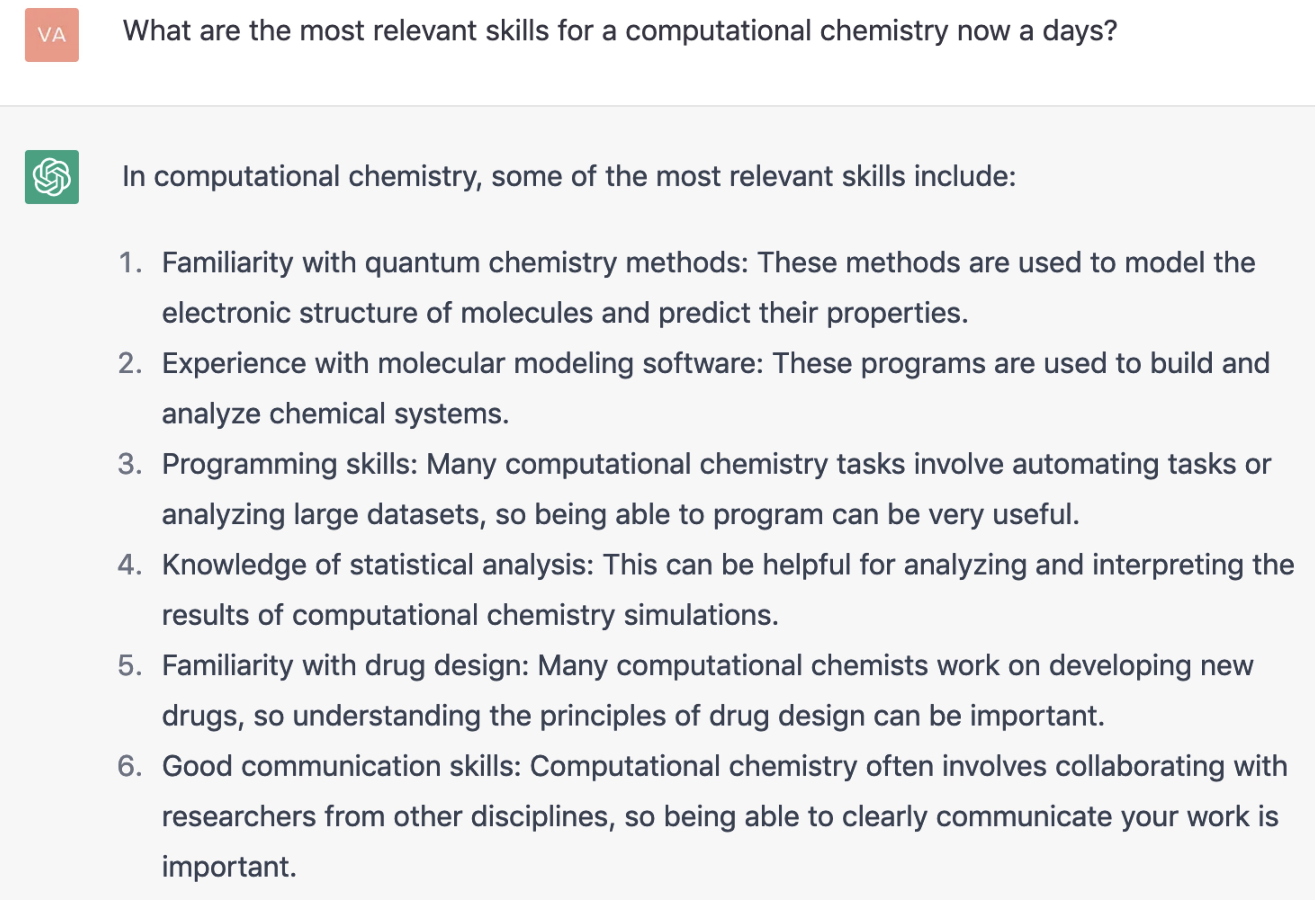
   ii. RDKit

   iii. **Molecular Dynamics**: JaxMD, TorchMD, openMD

   iv. **Visualization**

What do you want to learn?

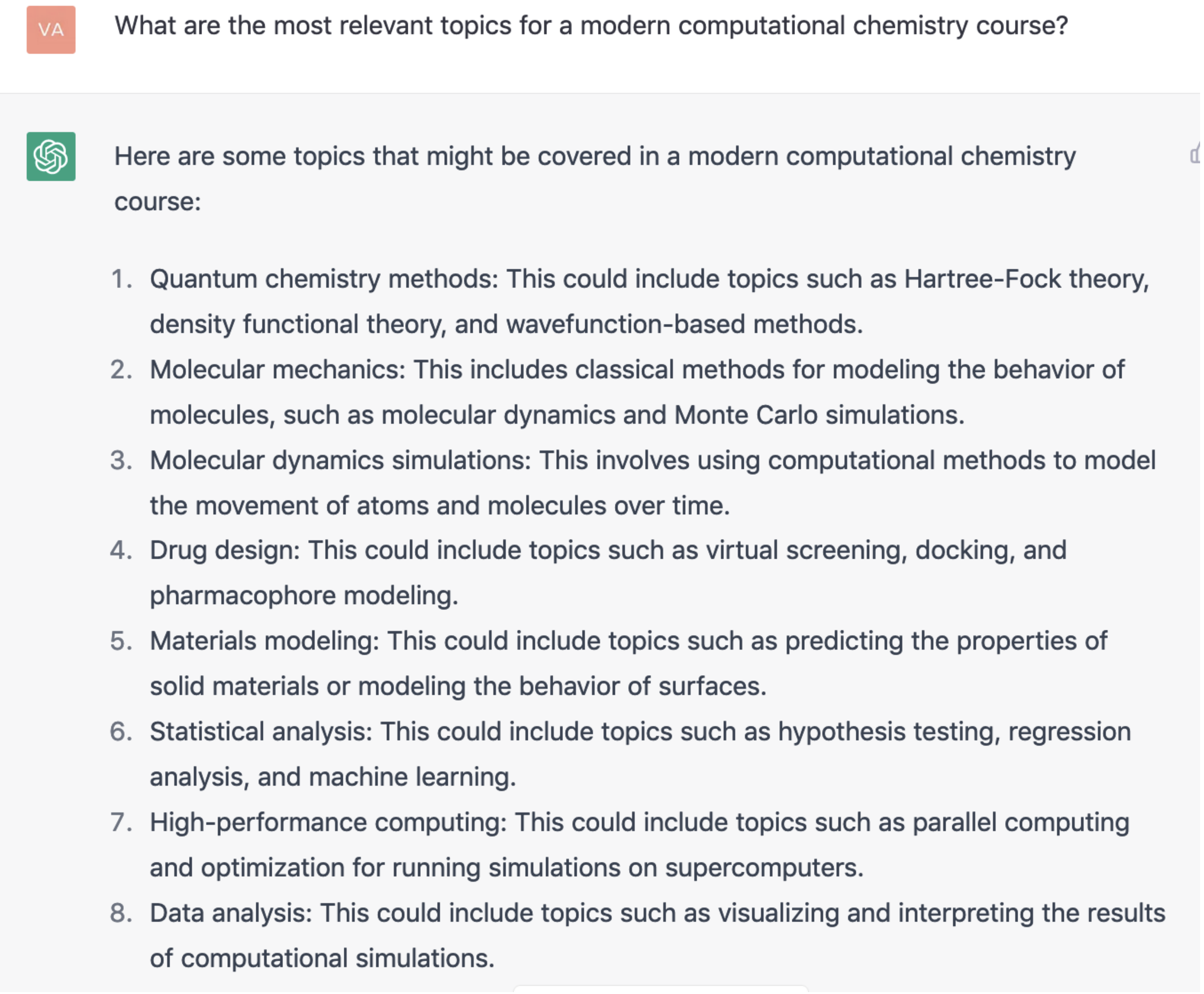
- This course is for you!



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.



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.