A Physical Chemistry course for non-Physical Chemists. Active learning strategies using Python and Jupyter Notebooks.

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Highlights

- *A one-semester survey Physical Chemistry course for everyone.*
- *Optionally followed by a more rigorous second semester for future physical chemists.*
- *Using molecular thermodynamics approach: Overview of quantum mechanics, spectroscopy, statistical thermodynamics, and macroscopic thermodynamics.*
- *Focusing on graphical representation and interpretation of solutions and not mathematical demonstrations.*
- *Using open-source software students can run all activities on their laptops during class.*
- *Python Conda environment with Jupyter, Matplotlib, Numpy, Simpy, Pandas, PSI4, OpenMM*
- *Not a coding class: Rather than asking students to produce their own code, they start by understanding and modifying code given to them to investigate the physical magnitudes affecting the properties of matter.*
- *Class time spent mostly activities in Jupyter: modify Python code to build and interpret tables and plots.*
- *Activities available at https://github.com/xavierprat/Physical-Chemistry-with-Jupyter*
- *Bridging analytical and computational solutions: Using computational chemistry tools (PSI4) and molecular simulation software (OpenMM) when the solution is not analytical.*

Topics: mixing analytical and computational approaches

Bohr's H atom → Quantum Particle in a Box → Schrodinger's Hydrogen atom → Polyelectronic atoms: SCF → Electronic structure of molecules → Molecular structure optimization → Molecular Vibrations and Rotations → Boltzmann factors → Partition functions of ideal systems → Molecular dynamics of real systems → Thermodynamics of real systems

Class structure: mixing lecture and practice everyday

In class: all students have laptops with conda environment

Start by presenting the main concepts and theories. Instructor gives Jupyter Notebook covering all the theory and scripts. Show a Python script plotting the law or table with results.

1) Students run the Jupyter cell. Explain the code by interpreting what each line does

2) Investigate with plots and tables how physical magnitudes affect properties of matter

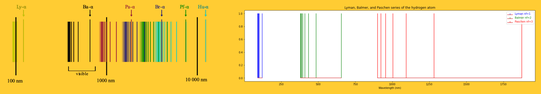
Homework: turn in Jupyter Notebooks

3) Modify the given Python scripts to new systems and extract conclusions.

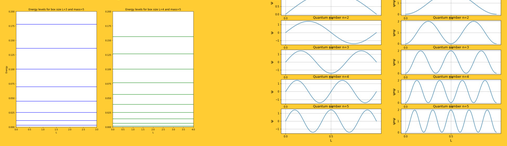
4) Optional challenge with writing new Python code

Classroom activities

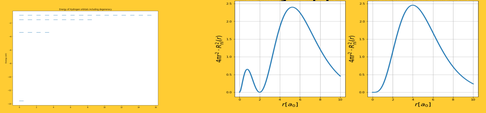
Bohr's atom:
Reproduce the emission spectrum of hydrogen



Particle in a box:
Investigate the quantum/classical limit: effect of mass and size of the box. Explore meaning of wavefunction, and degeneracy of levels



Schrodinger's Hydrogen atom:
Plot energy levels and radial probability distribution. See how Aufbau rules naturally appear



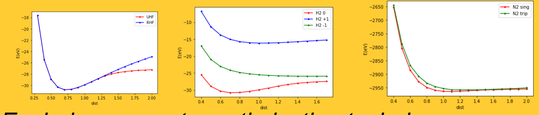
Use sympy and plotly for plotting the solution polynomials and use cutoff criteria to represent 3D orbitals

Polyelectronic atoms:
Using PSI4 for SCF calculations. Reproduce ionization energies in the periodic table

	First Ioniz(eV)	Second Ioniz(eV)
sct/sto-3g	4.900182	74.218914
b3lyp/sto-3g	5.263547	75.546576
scf/6-31G**	5.328965	75.662444
b3lyp/6-31G**	5.617527	77.084126
Experiment	5.390000	75.640000

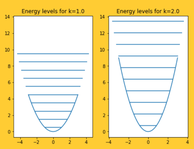
	First Ioniz(eV)	Second Ioniz(eV)
Li	5.328965	75.662444
Be	7.929997	18.115214
B	7.836308	23.453604
C	10.715420	24.159913

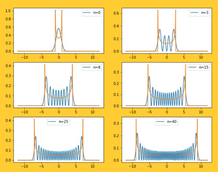
Electronic Levels of molecules:
Dissociation curves for different electronic states and charges of diatomic molecules



Exploring geometry optimization techniques.

Vibrational levels:
Investigate effect of mass and force constant on vibrational energy levels. Compare classical with quantum vibrational motion.

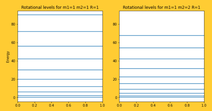




Calculate force constants of diatomic molecules and predict infrared spectroscopy.

Classroom activities

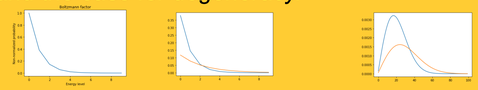
Rotational levels:
Investigating the effect of mass and bond distance on the energy levels of the rigid rotor. Rotational levels of real molecules



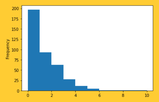
Eigenvalue J	CO	N2	O2	F2	NO
0	0.000000	0.000000	0.000000	0.000000	0.000000
1	0.096393	0.118064	0.085377	0.052947	0.101269
2	0.289180	0.354191	0.256130	0.158840	0.303808
3	0.578359	0.708383	0.512260	0.317680	0.607615
4	0.963932	1.180638	0.853767	0.529466	1.012692
5	1.445899	1.770956	1.280650	0.794199	1.519039
6	2.024258	2.479339	1.792910	1.111879	2.126654
7	2.699011	3.305785	2.390547	1.482505	2.835539
8	3.470157	4.250295	3.073561	1.906278	3.645680
9	4.337696	5.312969	3.841951	2.382598	4.557116

Predict rotational spectra using the $\Delta J = \pm 1$

Boltzmann factor
Compare the Boltzmann factor of different vibrational levels. Investigate effect of temperature and energy gap and the case for degeneracy.



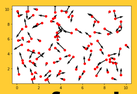
The money game emulates Boltzmann
Simulate if many students were to exchange $1 bill and find how final distribution matches Boltzmann



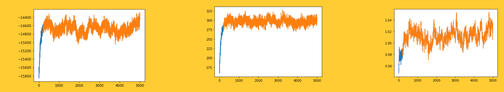
From *J. Chem. Educ.* 2006, 83, 4, 581

Partition function and Thermodynamic prop
Use PSI4 to calculate the electronic, vibrational, rotational, and translational contributions of many diatomic molecules and analyze them.

Introduction to molecular dynamics
The problem of non-ideal systems. Write a simple MD algorithm to converge the phase space of non-interacting particles.

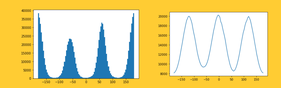


Thermodynamics of real systems
Simulate a Lennard-Jones liquid. Plot potential and kinetic energy. Simulate a box of waters using OpenMM. Calculate water heat capacity using energy fluctuations.

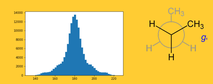


Water potential energy, Temperature, and density

Calculate the free energy (PMF) for the conformational rotation of ethane and butane. Investigate the effect of temperature, barrier, and time of simulation to converge a rare event.



Ethane 5 ns



Butane 5 ns

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