Python for Chemistry

Course Syllabus

Course Code: CHEM 485
Credits: 3
Instructor: Dr. Burhan Beycan
Duration: 14 weeks
Prerequisites: General Chemistry, Basic Programming Knowledge

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Course Description

This course introduces Python programming specifically tailored for chemistry applications. Students will learn to use Python for chemical calculations, data analysis, molecular modeling, and laboratory data processing. The course emphasizes practical applications in computational chemistry, spectroscopic data analysis, and chemical informatics.

Learning Objectives

Upon completion of this course, students will be able to:

1. **Master Python fundamentals** for scientific computing in chemistry
2. **Analyze chemical data** using NumPy, Pandas, and SciPy libraries
3. **Visualize molecular structures** and chemical properties using specialized libraries
4. **Process spectroscopic data** from NMR, IR, and UV-Vis instruments
5. **Implement chemical calculations** for thermodynamics, kinetics, and quantum chemistry
6. **Develop automated workflows** for laboratory data analysis

Course Outline

Week 1-2: Python Fundamentals for Scientists

- Python syntax and data types
- Control structures and functions
- Scientific computing environment setup
- Introduction to Jupyter notebooks

Week 3-4: Mathematical Operations in Chemistry

- NumPy for numerical calculations
- Chemical unit conversions
- Stoichiometric calculations
- Error propagation analysis

Week 5-6: Data Handling and Analysis

- Pandas for chemical datasets
- Reading laboratory data files
- Statistical analysis of experimental results
- Data cleaning and preprocessing

Week 7-8: Molecular Visualization and Modeling

- RDKit for molecular informatics
- 3D molecular visualization with Py3Dmol
- SMILES and molecular descriptors
- Chemical database queries

Week 9-10: Spectroscopic Data Analysis

- Processing NMR spectra

- IR and UV-Vis data analysis
- Peak detection and integration
- Spectral database comparisons

Week 11-12: Thermodynamics and Kinetics

- Chemical equilibrium calculations
- Reaction rate analysis
- Arrhenius equation fitting
- Phase diagram construction

Week 13-14: Advanced Applications

- Quantum chemistry interfaces (PySCF)
- Machine learning for chemical properties
- Automated report generation
- Final project presentations

Assessment Methods

Component	Weight	Description
Laboratory Assignments	40%	Weekly programming exercises
Midterm Project	25%	Spectroscopic data analysis project
Final Project	25%	Comprehensive chemical modeling project
Participation	10%	Class engagement and peer reviews

Required Software

- **Python 3.8+** with Anaconda distribution
- **Jupyter Notebook** or JupyterLab

- **RDKit** for cheminformatics
- **Matplotlib/Plotly** for visualization
- **SciPy ecosystem** (NumPy, Pandas, SciPy)

Textbooks and Resources

Primary Textbook

- **"Python Scripting for Computational Science"** by Hans Petter Langtangen
- **"Effective Computation in Physics"** by Anthony Scopatz & Kathryn Huff

Supplementary Resources

- RDKit Documentation and Tutorials
- Python for Chemists online resources
- Computational Chemistry Python (cclib) documentation

Laboratory Projects

Project 1: Molecular Property Calculator

Develop a Python program to calculate molecular properties from SMILES strings, including molecular weight, logP, and topological descriptors.

Project 2: Spectral Data Processor

Create an automated pipeline for processing and analyzing NMR or IR spectroscopic data, including peak picking and compound identification.

Project 3: Chemical Kinetics Analyzer

Build a comprehensive tool for analyzing reaction kinetics data, determining rate constants, and predicting reaction mechanisms.

Final Project: Integrated Chemical Informatics Platform

Design and implement a complete chemical informatics solution combining molecular modeling, data analysis, and visualization capabilities.

Grading Scale

Grade	Percentage	Description
A	90-100%	Excellent understanding and application
B	80-89%	Good grasp of concepts with minor gaps
C	70-79%	Satisfactory performance with some weaknesses
D	60-69%	Below average, significant improvement needed
F	<60%	Unsatisfactory performance

Course Policies

Attendance Policy

Regular attendance is essential for success in this hands-on course. More than two unexcused absences may result in grade reduction.

Late Assignment Policy

Late assignments will be penalized 10% per day unless prior arrangements are made with the instructor.

Academic Integrity

All work must be original. Collaboration is encouraged for learning, but submitted work must be individually completed.

Accommodation Statement

Students with documented disabilities should contact the Office of Disability Services to arrange appropriate accommodations.

Contact Information:
Dr. Burhan Beycan
Email: burhanbeycan@hotmail.com
Office Hours: Tuesdays and Thursdays, 2:00-4:00 PM
Location: Chemistry Building, Room 245