

11220CHEM528500 Python for chemists (Python 在化學上的應用)

Instructor: Prof. Tzuhsiung Yang (楊自雄). Office: R409

Date: 2/19(M) to 6/24(M); **Time:** R5R6, Thursday 13:20-15:10; **Location:** Chemistry R114

Language: English (may mix with Mandarin)

Course description: This is a Python course tailored for chemists with special focus on its application in various subfields of chemistry and daily routines of chemists.

Suggested textbooks:

1. 洪維恩，《Python 教學手冊》，ISBN 9789863126881，出版社：旗標科技股份有限公司
2. Mark Summerfield, Programming in Python 3: A Complete Introduction to the Python Language, Second Edition, Addison-Wesley, 2010, Person Education, Inc., Boston, MA USA.

Grading: Grades will be based on 1) attendance (10%), 2) midterm presentation (40%), and 3) a final project (50%).

Rule for the use of AI: LLM is an indispensable part of coding now. The use of LLMs like (ChatGPT) is allowed in this class. HOWEVER, you are required to know what code lines do.

Syllabus

Date	Class Week	Materials
22-Feb	1	Syllabus, Bash basics, IDEs
1-Feb	2	Python basics
7-Mar	3	Python basics
14-Mar	4	Pandas: The Python version of Excel
21-Mar	5	Make your own ChemFinder with RDKit and Pandas
28-Mar	6	Extract PDF and PNG with OpenCV and Textract
4-Apr	No class	
11-Apr	7	Midterm presentation
18-Apr	8	Midterm presentation
25-Apr	9	Make better figures with Matplotlib , Seaborn , and Plotly
2-May	10	Analyze your data and spectra with Numpy and Scipy
9-May	11	Website scrapping with Requests and BeautifulSoup
16-May	12	Python for materials science: Materials Project API
23-May	13	Python for protein: AlphaFold2 and Autodock Vina
30-May	14	Train a LLM (Like ChatGPT) for your research
7-Jun	15	Final presentation
13-Jun	16	Final presentation
20-Jun	17	Buffer week