



## 教學計劃表 Syllabus

課程名稱(中文) Course Name in Chinese	計算化學		學年/學期 Academic Year/Semester	114/2
課程名稱(英文) Course Name in English	Computational Chemistry			
科目代碼 Course Code	CHEM53800	系級 Department & Year	碩士	開課單位 Course-Offering Department
修別 Type	選修 Elective	學分數/時間 Credit(s)/Hour(s)	3.0/3.0	
授課教師 Instructor	/梁剛荐			
先修課程 Prerequisite				
課程描述 Course Description				
Python applications in computational chemistry				
課程目標 Course Objectives				
介紹目前在化學研究上，經常被使用之電腦程式及其在化學研究之應				
系專業能力 Basic Learning Outcomes				課程目標與系專業能力相關性 Correlation between Course Objectives and Dept.'s Education Objectives
A	具備化學專業知識			●
B	具備獨立思考及分析解決問題之能力			●
C	具備設計與執行化學實驗之能			○
D	具備國際視野與外語能			○
圖示說明Illustration : ● 高度相關 Highly correlated ○ 中度相關 Moderately correlated				
授課進度表 Teaching Schedule & Content				
週次Week	內容 Subject/Topics			備註Remarks
1	Introduction			
2	What is Computation			
3	Branching and Iteration			
4	Branching and Iteration			
5	String Manipulation, Guess and Check, Approximations, Bisection			
6	String Manipulation, Guess and Check, Approximations, Bisection			
7	Decomposition, Abstraction, and Functions			
8	Decomposition, Abstraction, and Functions			

9	Assignment 1	
10	Tuples, Lists, Aliasing, Mutability, and Cloning	
11	Recursion and Dictionaries	
12	Testing, Debugging, Exceptions, and Assertions	
13	Object Oriented Programming	
14	Object Oriented Programming	
15	Python Classes and Inheritance	
16	Assignment 2	
17		
18		

### 教學策略 Teaching Strategies

- 課堂講授 Lecture
  分組討論 Group Discussion
  參觀實習 Field Trip  
 其他 Miscellaneous:

### 教學創新自評 Teaching Self-Evaluation

#### 創新教學 (Innovative Teaching)

- 問題導向學習 (PBL)
  團體合作學習 (TBL)
  解決導向學習 (SBL)  
 翻轉教室 Flipped Classroom
  磨課師 Moocs

#### 社會責任 (Social Responsibility)

- 在地實踐 Community Practice
  產學合作 Industry-Academia Cooperation

#### 跨域合作 (Transdisciplinary Projects)

- 跨界教學 Transdisciplinary Teaching
  跨院系教學 Inter-collegiate Teaching

- 業師合授 Courses Co-taught with Industry Practitioners

其它 other:

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學期成績計算及多元評量方式 Grading & Assessments

配分項目 Items	配分比例 Percentage	多元評量方式 Assessments							
		測驗 會考	實作 觀察	口頭 發表	專題 研究	創作 展演	卷宗 評量	證照 檢定	其他
平時成績(含出缺席) General Performance (Attendance Record)									
期中考成績 Midterm Exam									
期末考成績 Final Exam									
作業成績 Homework and/or Assignments	100%	✓	✓						
其他 Miscellaneous (_____)									

評量方式補充說明

Grading & Assessments Supplemental instructions

教科書與參考書目 (書名、作者、書局、代理商、說明)

Textbook & Other References (Title, Author, Publisher, Agents, Remarks, etc.)

Introduction to Computation and Programming Using Python with Application to Understanding Data, 2nd Edition

課程教材網址(含線上教學資訊, 教師個人網址請列位於本校內之網址)

Teaching Aids & Teacher's Website(Including online teaching information.

Personal website can be listed here.)

<https://ocw.mit.edu/courses/electrical-engineering-and-computer-science/6-0001-introduction-to-computer-science-and-programming-in-python-fall-2016/lecture-videos/>

其他補充說明 (Supplemental instructions)