國立清華大學課程大綱 Syllabus

科號 Course Number	5004	學分 Credit	1	人數限制 Class Size	20
中文名稱 Course Title	分子模擬與建模二				
英文名稱 Course English Title	Molecular Simulation and Modeling II				
任課教師 Instructor	竹村　和浩 (TAKEMURA, Kazhiro)				
上課時間 Time		上課教室 Room			

課程簡述(必填) (最多 500 個中文字) 本欄位資料會上傳教育部課程網

Brief Course Description (required)　(50-200 words if possible, up to 1000 letters

"Molecular Simulation and Modeling (and II)" is designed for students who need to understand the basics of molecular simulations. There is no doubt that molecular simulations have been widely used in scientific research. Thanks to hardware developments, available software, and good tutorials, molecular simulations are relatively easy to conduct. However, a lack of understanding of the methods prevents researchers from overcoming possible troubles and developing new methodologies. This course aims to deepen understanding of theories used in molecular simulation, mainly molecular dynamics simulations of biomolecules. The content covers not all but some popular concepts used in molecular simulations. "Molecular Simulation and Modeling II" is the sequel to the course "Molecular Simulation and Modeling". This course will provide supplementary information to further enhance your knowledge in the field of molecular simulation and modeling. While it is recommended to complete "Molecular Simulation and Modeling" prior to enrolling in this class, key concepts from the earlier course will be briefly reviewed to ensure a solid understanding of the material.

請輸入課程內容「中文暨英文關鍵字」至少 5 個, 每個關鍵字至多 20 個中文, 以半形逗點分隔 (必填)

Please fill in at least 5 course keywords (up to 40 letters for each keyword) and use commas to separate them.(required)

molecular dynamics simulation, statistical mechanics, solvation, binding, correlation functions

課程大綱 Detailed Course Syllabus

● **課程說明(Course Description)**

By the end of this course, students will be able to

- Explain how to model molecules and conduct simulations
- Explain some techniques used in molecular simulations
- Understand and explain the basic theory used in molecular simulation

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● **指定用書(Text Books)**

Lecture notes will be given in the class

● **參考書籍(References)**

Benoît Roux. “Computational Modeling and Simulations of Biomolecular Systems.” World Scientific Publishing Co. Pte. Ltd..
Michael P. Allen, Dominic J. Tildesley “Computer Simulation of Liquids”
Daan Frenkel, Berend Smit “Understanding Molecular Simulation: From Algorithms to Applications” (Computational Science Series, Vol 1)

● **教學方式(Teaching Method)**

Lectures

● **教學進度(Syllabus)**

The sequence of the following content may change throughout the duration of the course.

1. **Course overview and Brief Review of “Molecular Simulation and Modeling”**
2. **Integrator**

3. Constraints
4. Basics of Analytical Mechanics
5. Temperature Control
6. Pressure Control
7. Molecular Interactions
8. Long-range interactions
9. Coarse-grained Models
10. Enhanced sampling techniques 1
11. Enhanced sampling techniques 2
12. Free energy calculations 1
13. Free energy calculations 2
14. Physical Properties Obtained from Simulations 1
15. Physical Properties Obtained from Simulations 2
16. Transition Rates and Markov State Model

● 成績考核(Evaluation)

Report (60%)
Participation including question and answer during class (40%)

● 可連結之網頁位址 相關網頁(Personal Website)

● Course policy for AI usage

https://curricul.site.nthu.edu.tw/p/404-1208-248378.php?Lang=zh-tw
This course adopts the following policy:
• Conditionally open - Students must briefly explain how generative AI was used for topic ideation, sentence refinement, or structural reference in the footnotes of the title page or after the reference in their assignments or reports. If usage is discovered without proper disclosure, instructors, the institution, or relevant units (e.g. our class) have the right to reevaluate the assignment or report or withhold scores.