Syllabus of CHEM-761 (3 Credit Hours)

Computational Study of Condensed Matters: from Theories to Applications

(Fall 2019, Monday/Wednesday 4:30 – 5:45 PM in Bilger 335)

Instructor: Rui Sun (Bilger 245B, ruisun@hawaii.edu)

Suggested Reading: *Computer Simulation of Liquids*, M.P Allen and D. J. Tildesley, 2nd Edition, ISBN-13: 978-0198803201, ISBN-10: 0198803206
Physical Chemistry: A Molecular Approach, D. McQuarrie and J. Simon, 2nd Edition, ISBN-13: 978-0935702996, ISBN-10: 0935702997
Grokking Algorithms: An Illustrated Guide for Programmers and Other Curious People, Aditya Bhargava, ISBN-13: 978-1617292231, ISBN-10: 1617292230

Prerequisites: Please send me an email to discuss the prerequisites before registering.

Overview: This course introduces the theories and applications of computational study of condensed matters. The course covers the theories behind simulations of condensed matters, and you apply these theories by writing computer programs that mathematically model a system of interest and to process the result. Further, you will use state-of-the-art computer software to carry out simulations of real-life problems.

Course Outline: The following topics will be covered:

- Programming**:** This course is not about computer programing, so we'll only learn and use the features that we'll need.
- High performance computing
- Statistical mechanics
- Molecular dynamics simulation
- Data Visualization

Assessments: The learning outcomes will be assessed through homework, projects, and one midterm. There will be NO final exam.

Method of Assessments	Points
(10) Homework	30
(3) Projects	45
(1) Midterm	25

1. Homework (30 pts) – Homework will be assigned almost weekly (10 in total) and you will be given a about week to finish it. Each homework is worthy of 3 pts. Homework is deducted by 33% every 24 hours past the deadline. You can discuss the homework with other students; however, assignments must be finished and submitted independently. **Most of the homework will involve computer programing.**

2. Projects (45 pts) – There will be three projects (including one final project) that involve computer programing. Each project is worthy of 15 pts. Again, you can discuss the projects with other students; but the project report must be finished and submitted independently.

3. Midterm Exam (25 pts) – There will be one midterm exam. The questions on the exam will be based on the reading assignment and lecture note. The date of the midterms is to be announced. The midterm will be closed-book.

Grading Scheme: You will get partial credits for a reasonable attempt at each assessment. The sum of all the above will determine your final score, for which letter grades will be assigned (**A:** 85 pts or above; **B:** 70 ~ 84 pts; **C:** 55 ~ 69 pts; **F:** 54 pts or below).

Special Conditions: Any student who feels he/she may need an accommodation based on the impact of a disability is invited to contact me privately. I would be happy to work with you, and the KOKUA Program (Office for Students with Disabilities) to ensure reasonable accommodations in my course. KOKUA can be reached at (808) 956-7511 or (808) 956-7612 (voice/text) in room 013 of the Queen Lili'uokalani Center for Student Services.

Academic Honesty: It is the aim of the University to foster a spirit of complete honesty and high standard of integrity. Any attempt of cheating and plagiarism is regarded by the faculty and administration as a **most serious offense** and renders the offenders liable to serious consequences, possibly suspension. http://www.catalog.hawaii.edu/about-uh/campus-policies1.htm