Syllabus for CHEM 598
Molecular Modeling

Term:	Spring 2016	**Instructor:**	Dr. Jeffry D. Madura
Time:	MTh 3:00 PM - 5:00 PM	**Office:**	Mellon Hall 320
Room:	Fisher Hall 715	**Phone:**	(412) 396-4129
Credit Hours:	3	**E-mail:**	madura@duq.edu

Office Hour: by appointment

Text(s): Optional:

[1] Martin J. Field, *A practical introduction to the simulation of molecular systems*, Cambridge University Press, 1999.

[2] Daan Frenkel and Berend Smit, *Understanding molecular simulation*, 2nd ed., Academic Press, Inc., Orlando, FL, USA, 2001.

[3] H.D. Höltje and et al., *Molecular modeling*, Methods and principles in medicinal chemistry, Wiley, 2008.

[4] Brooks C. L. III, M. Karplus, and B. M. Pettit, *Proteins: A Theoretical Perspective of Dynamics, Structure & Thermodynamics*, Advances in Chemical Physics LXXI, Wiley, New York, 1988.

[5] Frank Jensen, *Introduction to computational chemistry*, John Wiley & Sons, 2006.

[6] Andreas Kukol, *Molecular Modeling of Proteins*, 2 ed., Methods in Molecular Biology, vol. 1215, Springer, September 2014.

[7] Andrew Leach, *Molecular Modelling: Principles and Applications (2nd Edition)*, 2 ed., Prentice Hall, April 2001.

[8] J. A. Mccammon and S. C. Harvey, *Dynamics of Proteins and Nucleic Acids.*, Cambridge Univ. Press, Cambridge, MA, 1987.

[9] A.K. Rappé and C.J. Casewit, *Molecular mechanics across chemistry*, University Science Books, 1997.

[10] Gregory A. Voth (ed.), *Coarse-Graining of Condensed Phase and Biomolecular Systems*, CRC Press, 2009.

Description: This is a knowledge and skills based course that covers a variety of molecular modeling topics. Topics to be covered include basic scripting, visualization, force-fields, molecular dynamics, enhanced sampling, docking, pharmacophores, free energy methods and drug design. Software to be used will include Python, LaTeX, MOE, VMD, NAMD, HTMD/acemd, and Gaussian.

Prerequisite(s): None.

Course Outline: We will use a series of papers as our reading material along with a molecular modeling document being written. The tentative list of topics includes:

- Basic computational skills
- Visualization
- Force-fields
- Electrostatics
- Molecular dynamics
- Protein dynamics
- Enhanced sampling methods
- Free Energy methods
- Docking / Virtual screening

This course syllabus provides a general plan for the course; deviations may be necessary.

- Homology modeling
- Drug design methods
- Soft matter
- Solid-state

Software to be used:

- Python
- LaTeX
- MOE
- VMD
- APBS
- NAMD
- HTMD/acemd
- Modeller
- SeeSAR / LeadIT
- WIEN2K
- Crystal14
- Gaussian09

January					February				
Mon	Tue	Wed	Thu	Fri	Mon	Tue	Wed	Thu	Fri
			7 Intro-duction	8	1 molecular dynamics	2	3	4 molecular dynamics	5
11 Visual-ation	12	13	14 force-field	15	8 protein dynamics	9	10	11 protein dynamics	12
18 MLK Day No Class	19	20	21 force-field	22	15 enhanced dynamics	16	17	18 FEP	19
25 electro-statics	26	27	28 electro-statics	29	22 FEP	23	24	25 docking	26
					29 Spring Break				
March					April				
Mon	Tue	Wed	Thu	Fri	Mon	Tue	Wed	Thu	Fri
	1 Spring Break	2 Spring Break	3 Spring Break	4 Spring Break					1
7 docking	8	9	10 homology	11	4 drug design	5	6	7 drug design	8
14 ACS No Class	15 ACS	16 ACS	17 homology	18	11 drug design	12	13	14 soft matter	15
21	22	23	24 Easter Break	25 Easter Break	18 soft matter	19	20	21 solid state	22
28 Easter Break	29	30 Mon. Sched. bind-site	31 ph4		25 Last Day solid state				

Attendance: Students are expected to attend class and arrive in a timely fashion.

Policy on Academic Honesty: All students are expected to abide by the policy on academic honesty of the *Bayer School of Natural and Environmental Sciences*.

Homework: Assignments will be turned in through Blackboard as a PDF. The naming convention for the PDF document will be your last name_first initial_assignment number.pdf, e.g. *madura_j_01.pdf*

In-Class Exams: This course will have no exams. In place of the exams there will be several assignments that will be given and graded. Each assignment will be worth 100 points.

Make-Up Policy: There will be no makeups on assignments.

Final Exam: There will be no final exam for this course.

Grades: I am anticipating approximately ten (10) assignments which means the course will have a total of 1000 points.

930-1000	93% to 100%	A
900-929	90% to 92.9%	A-
870-899	87% to 89.9%	B+
830-869	83% to 86.9%	B
800-829	80% - 82.9%	B-
770 - 799	77% to 79.9%	C+
769-700	70% to 76.9%	C
600-699	60% to 69.9%	D
0-599	$< 60\%$	F

The following describes what each grade represents.

A/A- Excellence overall, no major weakness. A-level work demonstrates real achievement in grasping what chemical thinking is, along with clear development of a range of specific chemical thinking skills or abilities. The work at the end of the course is, on whole, clear, precise, and well-reasoned, though with occasional lapses into weak reasoning. In A-level work, chemical thinking terms and distinctions are used effectively. The work demonstrates a mind beginning to take charge of its own ideas, assumptions, inferences, and intellectual processes. The A-level student usually analyzes issues clearly and precisely, usually formulates information clearly, usually distinguishes the relevant from the irrelevant, usually recognizes key questionable assumptions, usually clarifies key concepts effectively, typically uses language in keeping with educated usage, frequently identifies relevant competing points of view, and shows a general tendency to reason carefully from clearly stated premises as well as noticeable sensitivity to important implications and consequences. A-level work displays excellent reasoning and problem-solving skills. The A-student's work is consistently at a high level of intellectual excellence.

B+/B/B- The essence of B-level work is that it demonstrates more strengths than weaknesses and is more consistent in high level performance than C-level work. It nevertheless has some distinctive weaknesses though no major ones. B-level work represents demonstrable achievement in grasping what chemical thinking is, along with the clear demonstration of a range of specific chemical thinking skills or abilities. B-level work at the end of the course is, on the whole, clear, precise, and well-reasoned, though with occasional lapses into weak reasoning. On the whole, chemical thinking terms and distinctions are used effectively. The work demonstrates a mind beginning to take charge of its own ideas, assumptions, inferences, and intellectual processes. The student often analyzes issues clearly and precisely, often formulates information clearly, usually distinguishes the relevant from the irrelevant, often recognizes key questionable assumptions, usually clarifies key concepts effectively, typically uses language in keeping with educated usage, frequently identifies relevant competing points of view, and shows a general tendency to reason carefully from clearly stated premises, as well as noticeable sensitivity to important implications and consequences. B-level work displays good scientific reasoning and problem-solving skills.

C+/C The essence of C-level work is that it demonstrates more than a minimal level of skill, but it is also highly inconsistent with as many weaknesses as strengths. C-level work illustrates some bu t inconsistent achievements in grasping what chemical thinking is, along with the development of modest chemical

thinking skills or abilities. C-level work at the end of the course, it is try, shows some emerging chemical thinking skills, but also pronounced weaknesses as well. though some assignments are reasonably well done, others are poorly done; or at best are mediocre. There are more than occasional lapses in reasoning. Though chemical thinking terms and distinctions are sometimes used effectively, sometimes they are used quite ineffectively. Only on occasion does C-level work display a mind taking charge of its own ideas, assumptions, inferences, and intellectual processes. Only occasionally does C-level work display intellectual discipline and clarity. The C-level student only occasionally analyzes issues clearly and precisely, formulates information clearly, distinguishes the relevant from the irrelevant, recognizes key questionable assumptions, clarifies key concepts effectively, uses language in keeping with educated usage, identifies relevant competing points of view, and reasons carefully from clearly stated premises, or recognizes important implications and consequences. Sometimes the C-level student seems to be simply going through the motions of the assignment, carrying out the form without getting into the spirit of it. On the whole, C-level work shows only modest and inconsistent reasoning and problem-solving skills and sometimes displays weak reasoning and problem-solving skills.

D The essence of D-level work is that it demonstrates only a minimal level of understanding and skill in chemical thinking. D-level work shows only a minimal level of understanding of what chemical thinking is, along with the development of some, but very little, chemical thinking skills or abilities. D work at the end of the course, on the whole, shows only occasional chemical thinking skills, but frequent unscientific thinking. Most assignments are poorly done. There is little evidence that the student is 'reasoning" through the assignment in a scientific manner. Often the student seems to be merely going through the motions of the assignment, carrying out the form without getting into the spirit of it. D work rarely shows any effort to take charge of ideas, assumptions, inferences, and intellectual processes. In general, D-level thinking lacks discipline and clarity. In D-level work, the student rarely analyzes issues clearly and precisely, almost never clarifies key concepts effectively, frequently fails to use language in keeping with educated usage, only rarely identifies relevant competing points of view, and almost never reasons carefully from clearly stated premises, or recognizes important implications and consequences. D-level work does not show good scientific reasoning and problem-solving skills and frequently displays poor reasoning and problem-solving skills.

F The essence of F-level work is that the student demonstrated a pattern of unscientific thinking and/or failed to do the required work of the course. Here are typical characteristics of the work of a student who receives an F. A close examination reveals: The student does not understand the basic nature of chemical thinking, and in any case does not display the chemical thinking skills and abilities which are at the heart of this course. The work at the end of the course is vague, imprecise, and unreasoned as it was in the beginning. There is little evidence that the student is genuinely engaged in the task of taking charge of his or her thinking. Many assignments appear to have been done pro forma, the student simply going through the motions without really putting any significant effort into thinking his or her way through them. Consequently, the student is not analyzing issues clearly, not formulating information clearly, not accurately distinguishing the relevant from the irrelevant, not identifying key questionable assumptions, not clarifying key concepts, not identifying relevant competing points of view, not reasoning carefully from clearly stated premises, or tracing implications and consequences. The student's work does not display discernable scientific reasoning and problem-solving skills.

Important Deadlines: Registration and add/drop ends January 12 . The last day to withdraw from the course is March 29 .

Student Disabilities Policy: If you have now or develop during this semester a physical or learning disability and you want your professor to make reasonable accommodations for that, you must contact the Office of Disability Services. Once the Office of Disability Services has received appropriate documentation, they will inform your instructor.