

Computational Chemistry

CHM 425/525-001
Office: Room 242E

Fall, 2011
Phone: 962-3453

Ned H. Martin
Email: martinn@uncw.edu

(LAB) Tu. 11:00 am-1:45 pm (DO 230) and (Lecture) Th. 11:00 am-12:15 pm (DO 230A)

<u>Date</u>	<u>Lecture topic (reading assignment) / LAB exercise (reading assignment)</u>
Th. Aug. 25	Introduction to computational chemistry
Tue. Aug. 30	Molecular mechanics, part 1 (<i>HyperChem manual</i> , Part I: Chapters 1, 2 & 3 pp 17-27; Part II: Chapter 1)
Th. Sept. 1	Molecular mechanics, part 2 (<i>HyperChem manual</i> , Part I: Chapters 4 & 7; Part II: Chapter 2)
Tue. Sept. 6	LAB 1. Building and optimizing structures in <i>Titan</i> (HSH lab book, Tutorial 1 and I. Computational Tools; <i>Titan manual</i> , Chapters 2-6)
Th. Sept. 8	Molecular orbital theory, part 1; <i>HyperChem manual</i> , Part I: Chapter 3 pp 27-43; Part II: Chapter 3)
Tue. Sept. 13	LAB 2. Manual conformation searching methods (HSH lab book, Tutorial 1, pp. 260-267 and II. Finding Molec. Geom)
Th. Sept. 15	<i>Ab Initio</i> MO Theory; Molecular orbital theory, part 2 (<i>HyperChem manual</i> , Part I: Chapter 8)
Tue. Sept. 20	LAB 3. Automated conformation searching (<i>HSH lab book</i> , Tutorial 2, pp. 268-276; <i>Titan manual</i> , Chapter 11)
Th. Sept. 22	Calculating molecular properties (<i>Titan manual</i> , Chapter 22; <i>HyperChem manual</i> , Part I, Chapter 8)
Tue. Sept. 27	LAB 4. Ring strain in cycloalkanes; isodesmic reactions (Exp't. 5, <i>HSH lab book</i> , III. <i>Isodesmic Reactions</i>) and take-home, open book TEST 1 (due Th. Oct. 6)
Th. Sept. 29	Electrostatic Effects: Computing charges on atoms (<i>HSH lab book</i> , V. <i>Charges on Atoms in Molecules</i>)
Tue. Oct. 4	LAB 5. Stability of alkenes and carbocations (<i>Titan manual</i> , Chapter 24)
Th. Oct. 6	Density Functional Theory: Dr. Lee Bartolotti, ECU (<i>HL df calc</i> , Chapters 1-4) TEST 1 due
Tue. Oct. 11	Fall Break; No Class
Th. Oct. 13	Potential energy surfaces; optimization methods; reaction path following; <i>Transition state modeling</i> (<i>HYKL mm and qc calc</i> , Chapter 5; <i>HyperChem manual</i> , Part I, Chapter 5; Part II, Chapter 4)
Tue. Oct. 18	LAB 6. Basicity of amines (Exp't. 40 <i>HSH lab book</i> , IV. <i>The Role of Solvent</i>)
Th. Oct. 20	Quantitative Structure-Activity Relationships (QSAR)
Tue. Oct. 25	LAB 7. Modeling bromonium ion intermediates (Exp't. 52)
Th. Oct. 27	Solvation effects; hybrid (QM/MM) methods
Tue. Nov. 1	LAB 8. Modeling a reaction pathway; the pinacol rearrangement (Exp't. 67 <i>HSH lab book</i> , XV. <i>Finding transition states</i> ; <i>Titan manual</i> , Chapter 9)
Th. Nov. 2	Modeling remote interactions
Tue. Nov. 8	LAB 9. Endo/Exo Selectivity in Diels-Alder Cycloadditions (Exp't. 77 <i>HSH lab book</i>)
Th. Nov. 10	UNIX / LINUX operating systems; remote computing; using Gaussian 03

- Tue. Nov. 15 LAB 10. Classical vs. Non-Classical Carbocations; NMR shift and charge calculations using *Gaussian 03* on a remote computer (lab counts double)
- Th. Nov. 17 TEST 2
- Tue. Nov. 22 LAB 11. Modeling the Relative Acidities of Substituted Phenols (*HSH lab book, IX. Graphical Models and Graphical Modeling*)
- Th. Nov. 24 Thanksgiving; No Classes
- Tue. Nov. 29 LAB 10 cont'd *Gaussian 03* on a remote computer
- Th. Dec 1 WWW Computational Chemistry Resources; Modeling Biomolecules
- Tue. Dec. 6 (12:15 pm) Oral Reports on LAB 10. NMR shift and charge calculations and Introduction to Molecular Dynamics and its Applications (Dr. Hee-Seung Lee)
- Tue. Dec. 13 FINAL EXAM 11:30 am – 2:30 pm DO-230A**

LAB reports are to be written in MSWord or (preferably) Excel and submitted as an attachment to email to martinn@uncw.edu no later than one week after the lab is scheduled. Each must be named as follows: the number of the lab experiment followed by your initials: e.g., **3nhm.xls** Ongoing efforts should be made to improve the readability/usability and appearance of the reports.

Grading:

15 Basic computational chemistry skills	60 points
2 Tests	200 points
11 Computational lab reports (#11 counts double)	120 points
Final Exam (comprehensive)	<u>120 points</u>
Total	500 points

(Graduate students must also complete a computational chemistry project with a written report)

90% = A 80% = B 70% = C 60% = D

Texts: (to be loaned to students by instructor; no text needs to be purchased)

HyperChem Computational Chemistry (*HyperChem manual*)

TITAN Tutorial and User's Guide (*Titan manual*), Wavefunction, Schrodinger, 1999

A Laboratory Book of Computational Organic Chemistry, (*HSH lab book*), Warren J. Hehre, Alan J. Shusterman, W. Wayne Huang, Wavefunction, Irvine, 1996.

A Brief Guide to Molecular Mechanics and Quantum Chemical Calculations, (*HYKL mm and qc calc*) Warren J. Hehre, Jianguo Yu, Philip E. Klunzinger, Liang Lou, Wavefunction, Irvine, 1997.

A Guide to Density Functional Calculations in Spartan, (*HL df calc*) Warren J. Hehre, Liang Lou, Wavefunction, Irvine, 1997.

Additional Resources (available in Randall Library):

Introduction to Computational Chemistry, Frank Jensen, Wiley, Chichester, 1999

Molecular Modeling: Perspectives and Applications, Andrew R. Leach, Addison Wesley Longman, Harlow, 1996

A Handbook of Computational Chemistry, Tim Clark, Wiley-Interscience, NY, 1985

Encyclopedia of Computational Chemistry, (Ref QD 39.3.) Ed. Paul v. R. Schleyer, Wiley, Chichester, 1998

Learning Outcomes:

Students are expected to have working knowledge of the language of computational chemistry, the various levels of theory (molecular mechanics, semi-empirical molecular orbital theory, ab initio molecular orbital theory, correlated methods, and density functional theory). The assessment measure of these outcomes is success on the hour tests and/or the final exam. Use of Titan software to perform fundamental operations in computational chemistry will be assessed by lab reports and by performance on the mastery skills tests.

Academic Integrity:

All members of UNCW's community are expected to follow the academic Honor Code. Please read the UNCW Honor Code carefully (as covered in the UNCW Student Handbook). Academic dishonesty in **any** form will not be tolerated in this class.

http://www.uncw.edu/policies/documents/03_100FINALHONORCODE_Aug2009.pdf

Students with Disabilities:

Students with diagnosed disabilities should contact the Office of Disability Services (962-7555). Please give me a copy of the letter you receive from Office of Disability Services detailing class accommodations you may need. If you require accommodation for test-taking please make sure I have the referral letter no less than three days before the test.

Violence and Harassment:

UNCW practices a zero tolerance policy for any kind of violent or harassing behavior. If you are experiencing an emergency of this type contact the police at 911 or UNCW CARE at 962-2273.

Resources for individuals concerned with a violent or harassing situation can be located at

<http://www.uncw.edu/wsrc/crisis.html>

Campus Respect Compact:

UNCW has recently instituted a Respect Compact to affirm our commitment to a civil community, characterized by mutual respect. That Compact will soon be affixed to the wall of each classroom and can be accessed at: <http://www.uncw.edu/stuaff/pdc/documents/SeahawkRespectCompact.pdf>

Individuals wanting more information about the respect Compact can contact the Office of Institutional Diversity and Inclusion.

Use of electronic devices during class:

Cell phone use will not be tolerated in this class. Turn off your cell phones prior to class. If your cell phone rings, Dr. Martin will answer it for you. You do not want this to happen. No ipods or other listening devices may be used during class or exams. Laptops may be used in this class, but only for following PowerPoint presentations or note-taking. No web surfing, texting or email access is allowed during class time.