CH E 491 – Special Topics: Calculation of Material and Molecular Properties

Fall Semester 2014

Classroom and Class Schedule: EC1 Room 210B, Tuesday & Thursday 10:20-11:35 AM

No class during AICHE meeting (Nov. 18 and 20) and Thanksgiving Holiday (Nov. 25 and 27).

Catalog Description:

CH E 491. Special Topics: Calculation of Material and Molecular Properties 3 cr.
The aim is to describe and apply techniques for computing common properties of materials and molecules: optimized geometries, transition states, vibrational spectra, energies (electronic, internal energy, enthalpy, and Gibbs free energy), heat capacities, net atomic charges, atomic spin moments, and effective bond orders. These techniques allow one to estimate the thermodynamic properties of a chemical, as well as to compute the mechanisms and energy barriers for chemical reactions and catalytic processes, and to quantify the electronic, magnetic, and chemical ordering in materials. The theory behind these techniques will be described and students will perform hands-on computer exercises using common computational chemistry programs. Prereq: CHEM 116, MATH192G, and (PHYS 214 or PHYS 216G)

Required Textbook: James Foresman and Aeleen Frisch, Exploring Chemistry with Electronic Structure Methods, Second Edition, Gaussian INC, ISBN 978-0-9636769-3-1.

Audience: This technical elective is intended for undergraduate and graduate students with a background in engineering, chemistry, physics, or materials science.

Instructor: Dr. Tom Manz
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Office hours: Monday 5-5:15 PM, Wednesday 5-5:15 PM, Friday 11:35 AM -12:00 PM

except Sept. 1 (Labor day), Nov. 17, 19, and 21 (AICHE annual meeting), Nov. 24, 26, and 28 (Thanksgiving Holiday).

Final Exam: 2 hours, comprehensive, EC1 Room 210B, Thursday Dec 11, 2014 from 10:30 AM – 12:30 PM

Topics Covered:

- Basic concepts of computational chemistry
- Calculating the energies and geometries of reactants and products for chemical reactions
- Finding the transition state of a chemical reaction: determining the reaction pathway, transition state geometry, and the energy barrier. Meaning of the energetic span for a catalytic cycle.
- Quantifying whether the transition state is closer to the reactant (early transition state) or closer to the product (late transition state). Postulates related to transition state lateness.
- Computing vibrational spectra
- Using the harmonic approximation to estimate thermodynamics properties: internal energy, enthalpy, Gibbs free energy, and heat capacities

- Computing net atomic charges, atomic spin moments, and effective bond orders to determine the electronic, magnetic, and chemical ordering of materials

Grading:

Attendance, 5 %

Reading and Review of Journal Articles and Book Chapters, 15 %

Computer Projects, 20 %

Quizzes, 15 %

Oral Presentation, 10 %

Midterm Exam, 15 %

Final Exam, 20 %

The final exam will be two hours in length and will be **comprehensive**.

Late assignments may be turned in, but will be assigned a maximum of 60% credit. Assignments can be turned in early if a student expects to be absent.

Grading Scale:

90-100% A;
80-89% B;
70-79% C;
60-69% D;
below 60% F

Citation of sources in computer projects, oral presentation, and review of journal articles and book chapters: All figures taken from other sources must include a citation to the source in the figure caption. All references to data, statistics, scientific results and ideas must be cited. All sentences or paragraphs quoted verbatim must be included in quotations “” and the source indicated. No exceptions.

Online resource: Course related content will be posted on **canvas,** which is accessed via **nmsu.instructure.com.**

Withdrawals: Students **will not** receive an automatic drop for persistent absences or persistent failure to complete assignments. The responsibility for withdrawals is completely up to the student.

Working together on assignments:

Working with other students to learn the operation of computer programs and to understand the scientific concepts is encouraged. However, all assignments turned in by the student must show the **student's own work**. All examination answers must be **strictly one’s own work**. Copying assignments or allowing others to copy your assignments is strictly forbidden and both parties will receive a zero for the assignment. See the Common Syllabus Addendum for more details.

Incomplete Grades: A grade of Incomplete (I) is given **only if the student is passing** and cannot complete the required work for reasons beyond the student's control that develop after the last day to withdraw from the course.

Common Syllabus Addendum: This syllabus also contains the Department of Chemical Engineering, Common Syllabus Addendum, Spring 2014, that describes Attendance Policy, Disabilities, Misconduct, Re-grades, Student Work Products, Etiquette, Fundamental of Engineering Exam Supplied Reference Handbook, and Video Surveillance. This Common Syllabus Addendum can be found at http://chme.nmsu.edu/academics/syllabi/chme-common-syllabus-addendum/.