Christopher M. Hadad

(614) 688-3141 (voice)
(614) 292-1685 (fax)

hadad.1@osu.edu

Department of Chemistry
Newman and Wolfrom Laboratory
100 West 18th Avenue
Columbus, OH 43210-1185

www.chemistry.ohio-state.edu

March 18, 2008

Kathleen M. Hallihan, Ph.D.
Director, Curriculum and Assessment
Colleges of the Arts and Sciences
CAMPUS

Dear Kate:

The Department of Chemistry requests to create a new course at the undergraduate and graduate level in Nanochemistry (Chemistry 611).

The Nanochemistry course has been taught twice already by Professor James Coe (coe.1@osu.edu) in my department, each time as an experimental Chemistry 694 course. In these offerings, 13 or 17 students completed the course. Some of these students were from the College of Mathematical and Physical Sciences, and others were from disparate majors across the campus, including the College of Engineering.

The Chemistry Curriculum Committee has voted unanimously to create this course officially, and we await approval from the rest of the curriculum process.

Please let me know if you need anything further.

Sincerely,

Christopher M. Hadad
Professor of Chemistry
Vice Chair for Undergraduate Studies

The Ohio State University
Colleges of the Arts and Sciences New Course Request

Chemistry

Academic Unit

Chemistry

Book 3 Listing (e.g., Portuguese)

Nanochemistry

Number	Title		
611	Nanochemistry	G, UG	3
18-Character Title Abbreviation		Level	Credit Hours

Summer Autumn Winter Spring X Year 2009 (offered every other year)

Proposed effective date, choose one quarter and put an "X" after it; and fill in the year. See the OAA curriculum manual for deadlines.

A. Course Offerings Bulletin Information

Follow the instructions in the OAA curriculum manual. If this is a course with decimal subdivisions, then use one New Course Request form for the generic information that will apply to all subdivisions; and use separate forms for each new decimal subdivision, including on each form the information that is unique to that subdivision. If the course offered is less than a quarter or a term, please complete the Flexibly Scheduled/Off Campus/Workshop Request form.

Description (*not to exceed 25 words*): Introduction to fundamental concepts of nanoscience, exploring strategies for complex assemblies of molecules, and developing computational techniques for the investigation of nanotech structures.

Quarter offered: Spring Distribution of class time/contact hours: class MWF 48 min./ project on PCs

Quarter and contact/class time hours information should be omitted from Book 3 publication (yes or no): no

Prerequisite(s): CHEM 123

Exclusion or limiting clause: approval by instructor

Repeatable to a maximum of __0___ credit hours.

Cross-listed with:

Grade Option (Please check): Letter x S/U Progress ☐ What course is last in the series? __NA____

Honors Statement: Yes ☐ No ☒ GEC: Yes ☐ No ☒ Admission Condition

Off-Campus: Yes ☐ No ☒ EM: Yes ☐ No ☒ Course: Yes ☐ No ☒

Embedded Honors Statement: Yes ☐ No ☒

Service Learning Course*: Yes ☐ No ☒ *To learn more about this option, please visit http://artsandsciences.osu.edu/currofc/

Other General Course Information:

(e.g. "Taught in English." "Credit does not count toward BSBA degree.")

B. General Information

Subject Code____400501______________ Subsidy Level (V, G, T, B, M, D, or P)___BDM_____________________

If you have questions, please email Jed Dickhaut at dickhaut.1@osu.edu.

1. Provide the rationale for proposing this course:
   This course addresses the scientific basis of nanotechnology in lectures. While Engineering Depts. across the USA have nanotechnology courses, there is a lack of courses in MAPS that address the scientific basics. Students reinforce this perspective by learning to model a nanotech system of their choice with the Hyperchem software package by means of a sequence of homework assignments through the quarter culminating in a 10 min. presentation to the class.

2. Please list Majors/Minors affected by the creation of this new course. Attach revisions of all affected programs. This course is (check one): ☐ Required on major(s)/minor(s) ☐ A choice on major(s)/minors(s)
   x An elective within major(s)/minor(s) x A general elective:

3. Indicate the nature of the program adjustments, new funding, and/or withdrawals that make possible the implementation of this new course.
This course has been previously taught in the Sp. '05 and Sp. '07 by Dr. Coe as CHEM 694 course called Nanochemistry

4. Is the approval of this request contingent upon the approval of other course requests or curricular requests?

Yes ☐ No x List:

5. If this course is part of a sequence, list the number of the other course(s) in the sequence: No

6. Expected section size: 20 Proposed number of sections per year: 1

7. Do you want prerequisites enforced electronically (see OAA manual for what can be enforced)? Yes ☐ No x

8. This course has been discussed with and has the concurrence of the following academic units needing this course or with academic units having directly related interests (*List units and attach letters and/or forms*):
Not Applicable ☐
There were letters from Prof. Bhushan in Mechanical Engineering and the College of Engineering in '05 when this course was first offered.

9. **Attach a course syllabus that includes a topical outline of the course, student learning outcomes and/or course objectives, off-campus field experience, methods of evaluation, and other items as stated in the OAA curriculum manual and e-mail to asccurrofc@osu.edu.**

Approval Process The signatures on the lines in ALL CAPS (e.g. ACADEMIC UNIT) are required.

		Printed Name	Date
1.	Academic Unit Undergraduate Studies Committee Chair: [signature]	CHRISTOPHER HADAD	3/17/08
2.	Academic Unit Graduate Studies Committee Chair: [signature]	ROBERT COLEMAN	03/17/08
3.	**ACADEMIC UNIT CHAIR/DIRECTOR**: Malcolm M. Chisholm	M.H. Chisholm	3/17/08.

4. **After the Academic Unit Chair/Director signs the request, forward the form to the ASC Curriculum Office, 4132 Smith Lab, 174 West 18th Ave. or fax it to 688-5678. Attach the syllabus and any supporting documentation in an e-mail to asccurrofc@osu.edu. The ASC Curriculum Office will forward the request to the appropriate committee.**

		Printed Name	Date
5.	**COLLEGE CURRICULUM COMMITTEE**	**Printed Name**	**Date**
6.	**ARTS AND SCIENCES EXECUTIVE DEAN**	**Printed Name**	**Date**
7.	Graduate School (if appropriate)	Printed Name	Date
8.	University Honors Center (if appropriate)	Printed Name	Date
9.	Office of International Education (if appropriate)	Printed Name	Date
10.	**ACADEMIC AFFAIRS**	**Printed Name**	**Date**

Nanochemistry History

This course has been taught twice:

1) Spring ’05, CHEM 694, “Nanochemistry”, call # 20059-0, MWF 10:30-11:18 AM, 13 students finished
2) Spring ’07, CHEM 694, “Nanochemistry”, call # 21355-6, MWF 10:30-11:18 AM, 17 students finished

Grading

40% Homework – Homework problems are assigned in each of the first seven weeks (due one week later) that are designed to cover topics in nanoscience and introduce the computational tools used for the student’s modeling project .
35% Presentations – Each student picks a project of interest in nanotechnology from their own field or of their own interest. A 5 min. powerpoint presentation/proposal with 2 slides introduces the proposed projectto the class in the third week which is then modified in consultation with the lecturer so that the project has a chance of being accomplished with the tools at hand (Hyperchem, Spartan, Gaussian with Gaussview/ and corresponding tools at the Ohio Supercomputer Center), each student presents a 10 min. powerpoint presentation to the class on their modeling project in the 9^{th} or 10^{th} week. The presentations are graded by the TAs, Coe Group members, and the instructor.
25% Final – a traditional final is offered on the lecture materials.

’05 and ’07 Grade Breakdown

A	11	***********
A-	8	********
B+	4	****
B	5	*****
E	1	*

In the future, with more students, I expect the distribution to push to an average grade of “B” or “B+” including a few “C”s in the distribution.

Other materials included:
Syllabus from Spring ‘07
Course Poster with graphics of actual student projects.

Nanochemistry

CHEM 694: Nanochemistry, Dr. Coe, Spring 2007

course materials available on Carmen, https://carmen.osu.edu/

Course Description: This course is an advanced special study of nanochemistry. It addresses nanotech systems from an atomic and molecular perspective. It introduces fundamental concepts of nanoscience, explores current strategies for making complex assemblies of molecular components, and develops computational techniques for the investigation of these types of structures. Students will pick a nanotech system of interest and assignments will be related to developing a molecular model of that system with the Hyperchem software package. The course is intended for both senior undergrads and 1st year graduate students in various disciplines. Students will be taught how to use the modeling software (it is not prerequisite).

Disabilities: All students with documented disabilities, who need accommodations, should see the instructor privately to schedule an appointment as early in the quarter as possible. If your disability requires materials in alternative format, please contact the Office for Disability Services at 292-3307, Room 150 Pomerene Hall.

Time, Place, Call Number: MWF 10:30-11:18 AM in MP 2015, call# 21355-6, 3 credits

Lecturer: Dr. James V. Coe, Professor of Chemistry

- **Office Hours:** Wed. after class in EL 053, 11:30 AM to 12:30, or any time you can find me in my office. You may also check in lab (EL 027, 031, or 055).
- **Lecturer Phone:** office 292-9489, lab (EL 027) 292-1493, lab (EL031) 292-0089
- **Lecturer email:** coe.1@osu.edu

TA: Katherine Cilwa, office hours MW 11:30-12:30 in EL0031, kcilwa@chemistry.ohio-state.edu

Text: All reading materials are either available on this page (or will be xeroxed for the class). Powerpoint files of the lecture materials are also provided.

Weekly Topics:

Week 1) What is nanotechnology? Nanoscience basics, properties in the nanosize regime, scaling laws, clusters, Moore's law motivations, silicon chip limitations, nanotech hype

reading – Feynman's "There's Plenty of Room at the Bottom", and Drexler's Molecular Engineering, w1_nanotech_intro.ppt, w1_effect_of_size.ppt

homework – due Friday, March 30th - Choose a subject for investigation from the field of "Nanotechnology" of interest to you (or of interest in your major field of study). Send your TA, Katie Cilwa, an email with a few sentences describing and proposing a specific nanotech project. If we agree that this project is addressable with the tools at hand, then you will use this system for study with the Hyperchem program for later homework assignments and for a 5 min. presentation/proposal to the class in the 3rd week and a 10 min. presentation to the class in the 9th week.

Week 2) Computational basics for molecular modeling of nanoassemblies (using Hyperchem)

reading - Ken Rodriguez' Ch 2 review of computational chemistry, w2_computational_chemistry.ppt homework – due Friday April 6th, Katie Cilwa will assign a simple polyatomic molecule to each student (like methanol or water) and a larger polyatomic (like benzene or toluene) for submission to the Ohio Supercomputer Center. The molecule will be initially optimized using the Hyperchem program with the OPLS or MM molecular model, the PM3 semi-empirical method, ab initio HF theory with a 6-31G* basis set, and a hybrid DFT (B3LYP) with the 6/31-G* basis set. Report the results with a table of the optimized energy, the optimized geometry in terms of bond lengths and angles, the dipole moment, highest occupied molecular orbital, lowest unoccupied molecular orbital (if such properties are available from the method). Do a calculation of the vibrations at the HF/6-31G* level. Report each vibration with a sketch of the motions, vibrational frequency in cm^{-1}, and intensity in km/mol. Use Gaussian03 to do a few more advanced ab initio calculations on your polyatomic molecule starting with your optimized HF calculation from Hyperchem. Optimize your polyatomic at the MP2/6-31G* and CCSD(T)/6-31G* levels of theory. Report the same results and compare the total electronic energy of the HF, MP2, and CCSD(T) results. Learn how to submit a job on your assigned larger polyatomic molecule at the MP2/6-31G* level and submit it to Gaussian on the OSC supercomputer. Report the optimized geometry and IR vibrational spectrum.

Week 3) A first building block - single-walled-carbon-nanotubes (SWNTs), nanowires

reading – Merkle's Computational Nanotech, Molecular Bearings, Small World, Impossible, w3_carbon_SWNT.ppt

Brief Presentations – 5 min. presentation with 2 powerpoint slides which include the source, a description of the nanotechnology, and a look at the molecules involved. How big is the system? Is there a critical molecular part that could be treated with a high level theory? Can it be modeled? Motions? We will discuss merits of modeling.

homework, due April 13th, Katie Cilwa will assign a different [n,m] SWNT to each student in the class (n should be greater than or equal to 5). Make a pdb file of your [n,m] SWNT using Shaun William's programs (SWNT programs), Gaussview, and Hyperchem. This process will have been discussed in lecture. The program doesn't trim the tube, so in Hyperchem make it as uniform at the end as you can and terminate with H-atoms. Put the n and m value in the name of the *.pdb file and email the final *.pdb file to Katie Place a polyatomic molecule(s) inside the SWNT and email this *.pdb file to Katie, also. Find a pdb file from nanotech efforts on the internet and submit it to the TA electronically.

Week 4) Biochemistry is nanotechnology: complex assemblies from nature, protein strategies, modified biochemicals

reading – Smalley_vs_Drexler, http://www.rcsb.org/pdb/home/home.do, D. S. Goodsell, "Biomolecules and Nanotechnology", American Scientist 88(3) 230-237, May-June 2000. Not required, but good M. Gross, *Travels to the Nanoworld: Miniature Machinery in Nature and Technology* (Perseus, Cambridge, 1999) pp 3-109, w3_bio.ppt

homework due April 20nd – What is the Smalley/Drexler argument about? Summarize with a paragraph. Go to the Protein Data Bank, http://www.rcsb.org/pdb/home/home.do, download a protein's *.pdb file, input the file into hyperchem, how big is the protein in Daltons and in volume (use Hyperchem), what does this nanomachine do? Make an image of the protein with all atoms pictured and then with the just the ribbons (secondary structure), identify the protein's active region(s), identify the main structural features.

Week 5) Learning to simulate with Hyperchem. Building blocks of nanotechnology: self-assembled monolayers, nanoparticles, w5_SAMs.ppt

homework due April 27th - Make a movie of a nanotech building block crashing into another nanotech building block. Buckyballs and buckytubes work well for this. Do this at three different collision velocities. Extract 5 snapshots from each movie which show the subunits before, 3 snapshots during, and one after the collision. Report the velocity setup and the molecular model used. Hand in a page with 5 images and setup information for each of the three movies.

Week 6) Building blocks of nanotechnology: self-assembled monolayers, dendrimers, conductive polymers, nanoparticles, DNA, proteins, latex nanobeads, gold/metal/semiconductor nanoparticles and quantum dots. Reading - P. Avouris, J. Appenzeller, R. Martel, and S. J. Wind, "Carbon Nanotube Electronics", Proceedings of the IEEE, 91(11) 1772-1784, Nov. 2003, w6_nanoparticles.ppt, Dendrimers.ppt

homework due May 4th - 1) Build a 3x3x3 cube of NaCl unitcells using the Hyperchem crystal builder ("Database" menu, "crystals", choose samples). View this piece of the crystal perpendicular to the (1,0,0) and (1,1,1) Miller indices. Cut away half of the cube along the (1,1,1) plane such that the base of the remaining structure is the (1,1,1) plane. Capture and report an image of the structure. Report the distance from outer plane of atoms at the base [(1,1,1) plane] to the next closest plane and report the distance from the outer plane of atoms along the (1,0,0) plane to the next closest plane. 2) A structure of the 15 amino acid, membrane bound form of the small gramicidin protein is available for use with this problem in the Zipped Files Directory. It is called "gramicidin_1MAG.pdb". This protein is an antibiotic, i.e. it kills bacteria by destroying potassium ion gradients. Use Hyperchem's amino acid builder to build a structure as close to the "gramicidin_1MAG.pdb" structure as you can. You can open this structure and then build your protein next to it. The amino acid sequence of gramicidin is VAL GLY ALA *DLE ALA *DVA VAL *DVA TRP *DLE TRP *DLE TRP *DLE TRP. This protein is unusual in that it is not built entirely from "left handed" sterioisomers of the amino acids (some people don't call it a protein). The "D"s in the aminio acid names mean "dextarotary" (you must click a box at the bottom right of the amino acid builder to choose "L" or "D". Report a picture of your protein merged and aligned with "gramicidin_1MAG.pdb" in order to best show off the similarity. 3) Use the DNA builder to build a double-stranded DNA oligomer with ten As followed by 10 Ts on one of the strands. hand in a PDB file and a picture of the result. 4) Make a double-walled carbon nanotube that is about 16 Angstroms long with a [15,15] on the outside and a [10,10] on the inside. Use Hyperchem's periodic box to fill it with water. Leave the periodic box to the maximum dimensions perpendicular to the tube and make the periodic box 1.4 Angstroms longer than the tube in the tube dimension. To just get waters in the tube, select all the molecules, then deselect the two tubes and the inside waters, and then delete the green waters. This may serve as a simulation of flow through the tube next week. Render the inside waters with "ball and cylinder" while the carbon nanotubes are rendered as "sticks". Report two images of your box - one perpendicular to the tube and one looking down the tube.

Week 7) Nanotribology, SAMs, lubricant films, and biomolecule adhesion. Reading - Nanofabrication - G. M. Whitesides and J. C. Love, “The Art of Building Small” pp. 36-53 in *Understanding Nanotechnology* (WarnerBooks, 2002), w7_nanotech.ppt, w7_SAMS.ppt, w7_AFM_PFPE_Liu.ppt, w7_biomolecules.ppt

homework due May 11th - 1) Give the two primary reasons (from the Whitesides and Love article) why photolithography is limited for nanotechnology. 2) What is "soft lithography" and why is it called "soft"? 3) The polymer PDMS is often used in thin film projects including soft lithography. What is the chemical name of this polymer? Using Hyperchem, make a chain of it that is 5 monomers long and submit a *.jpg image of your result. 4) What is dip pen lithography and how does it work? 5) What is meant by "top down" vs "bottom up" methods in nanotechnology? 6) Submit a "*.hin" file indicating the present state of the model for your presentation project. Presentations start in week 9 and 10.

Week 8) Molecular electronics, single molecule switching devices, diodes, transistors. Reading - J. M. Seminario, L. E. Cordova, and P. A. Derosa, “An Ab Initio Approach to the Calculation of Current-Voltage Characteristics of Programmable Molecular Devices”, Proceedings of the IEEE, 91(11) 1958-1975, Nov. 2003. Shaun William's w8_molecular_electronics.ppt and w8_molecular_electronics.pdf, molecular_electronic_nano_051605.pdf

Week 9-10) ~10 min. presentations of molecular modeling and objectives of your nanoassemblies using PC. Nanomachines, motors, levers, gears, ratchets and transport.

Final Exam: Monday June 4th, 9:30-11:18 AM. As an alternative, you may write a final exam (due May 30th, to be graded by Dr. Coe) instead of taking the final.

Grading: Homework 40%, Presentations 35%, Final 25%.

Hyperchem and Gaussian: Homework and lectures will be augmented with the user-friendly commercial program Hyperchem. There are two PCs in EL0051 with Hyperchem 7.5, Gaussian03, and Gaussview. An full power evaluation copy of Hyperchem is available that works for 10 days, HyperChem751Evaluation.zip. The older evaluation copy might work (it was good for 30 days), HyperChem752Evaluation.zip. Gaussian03 and Gaussview are licensed on campus for PCs if you belong to a research group. You can get each program on a CD for $5 each with a 100W purchase order at 512 Baker Systems Engineering. Each member of this class has an Ohio Supercomputer Center account set up to use Gaussian03 on a supercomputer.

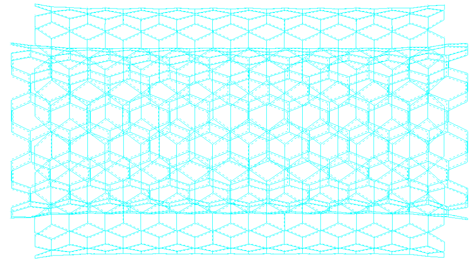
Building block molecules Zipped Files Directory

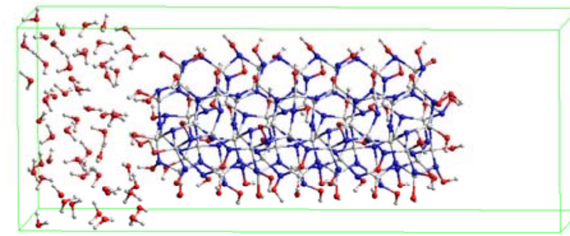
Secure Shell for accessing OSC computers sshwin3_29.zip

Spring 2007

Nanochemistry

Dr. Coe, CHEM 694, Call # 21355-6,
MWF 10:30-11:18 MP 2015





This course introduces fundamental concepts of nanoscience, explores current strategies for making complex assemblies of molecular components, and develops computational techniques for the investigation of these types of structures. Students will pick a nanotech system of interest and assignments will be related to developing a molecular model of that system with the Hyperchem software package. The course is intended for both senior undergrads and 1st year graduate students in various disciplines. Students will be taught how to use the modeling software (it is not prerequisite).

Student Projects