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Administrative Boards of the College of Arts and Sciences
Office of General Education
UNC-CH

Dear Colleagues:

NCSU Summer Program: Hangzhou Physical Chemistry & Research

This letter is to seek approval for the North Carolina State University Hangzhou Summer Program in **Physical Chemistry & Research**, based at Zhejiang University in the city of Hangzhou, China.

The establishment of this program is supported by the Department of Chemistry.

The program is led by Dr. Stefan Franzen, Professor at North Carolina State University in Biophysical and Biological Chemistry (PhD Stanford University). The program will run for 7 weeks from mid-May to late-June/early July. Prof. Franzen has led students to China several times and speaks Chinese. More information can be found on the program website:
http://chsfpc5.chem.ncsu.edu/~franzen/China/china.htm

Rationale
For the pool of science students who have very strict sequential major requirements to stay on track for graduation, this program gives those students the necessary academic content, while at the same time allowing them to immerse in a rich cultural experience. A site visit was completed by Dan Gold, Asian Programs Director, in July 2010. During his visit, he spoke with all programs participants and staff and was satisfied that students were able to successfully navigate life on a daily basis and have a rewarding cultural experience without formal Chinese language background or training, especially given the close participation of local students and faculty and the constant support and encouragement of the Resident Director. Through participation in the program's intense Chemistry curriculum, participants work daily with local students and faculty, giving them in-depth Chinese cultural immersion within their own academic context and environment. In addition, the students are given some training in survival Chinese while in Hangzhou.

Academics
While on this semester program, students take two courses (syllabi attached):

1. Physical Chemistry CH431 OR Physical Chemistry CH433 (depending on the student's level). Each class will confer 3 hours of TREQ transfer credit. For each class, students receive 37.5 hours of lecture and 22.5 hours of recitation (hands-on instruction in problem solving and review).

AND

2. CH499: Research in Computational Chemistry (will confer 3 hours of TREQ transfer credit). To obtain credit, students will need to spend a minimum of 135 hours in the lab. They have the option of doing some of the labwork in the summer when they return (to be supervised by Professor Franzen--either in his lab at NCSU or if they were able to find appropriate space at UNC).

The UNC Department of Chemistry will grant major credit as follows: UNC Course CHEM 482 (quantum mechanics) for CH431; UNC Course CHEM 481 (thermodynamics) for CH433; UNC Course CHEM 481L (2 credits) for CH499. The additional credit hour of CH499 will transfer back as general elective credit.

The core educational activity will be a Physical Chemistry course. The course will have a main lecture series complemented with breakout sessions to permit a separate focus for Biochemistry, Chemistry or Engineering students. In addition, a research project in computational chemistry will permit students to work with Chinese graduate students in a project that will train students in current methods.

Both courses will be taught by Prof. Franzen, assisted by two NCSU graduate TAs. Program participants will be joined by local students in their classes and will be joined by local faculty for some activities: Professor Wang Qi of the Chemistry Department will sponsor research activities in the area of ligand-receptor interactions and peroxidase catalysis. Professor Li Haoran will sponsor research in oxidation catalysis.

Full information on courses can be found at: http://chsfpc5.chem.ncsu.edu/~franzen/China/courses.htm.

Program logistics and location

The city of Hangzhou, with a population of about 7 million, is the capital of Zhejiang province. It is located about 1.5 hours south of Shanghai on the east coast of China. It serves as a political, economic and cultural center. It is home to the West Lake, one of the biggest tourist attractions in all of China, and hundreds of temples, historical sites, and tea plantations.

The program is based at Zhejiang University, which is generally regarded as one of the top 5 universities in China. Program residence will be in the International College of Zhejiang University located on the Yuquan campus just west of the city center and within walking distance of the West Lake. The International College hosts a variety of international academic programs in the summer.

Program participants will be housed in private doubles with attached bathrooms in the International College on campus. Facilities include classrooms, dining facilities and laundry as well as an international office which supports international students on-site. Western medical facilities on and nearby campus have been identified by the international office and the Program Director in case of illness and emergencies. There are additional student cafeterias across the campus as well as a convenience store.

The program will start in Beijing, visiting key historic sites in the city for 2-3 days before moving to Hangzhou for the program orientation at Zhejiang University. Following orientation, classes will meet daily for the remainder of the program. Weekend tours to local sites, and one additional weekend trip to a site such as the Yellow Mountains will be included. Throughout the term, local cultural and social events will also be scheduled to help acclimate students to local life and society.

On-site administration for the duration of the program will be handled by the Program Director, Prof. Franzen and two Chemistry Graduate Student TAs, who will live at the same location as the students.

For our students, there is a minimum GPA requirement of 3.0. In addition, all students must have met the

pre- or corequisites for the UNC Course CHEM 481 (CHEM 102 or 102H, PHYS 116, MATH 383, PHYS 117: C- or better) before attending this program. There is no language requirement.

We are happy to provide any further information that you may need to evaluate this proposal.

Yours sincerely:

Matthew Redinbo
Chair of Chemistry

Bob Miles
Associate Dean: Study Abroad and International Exchanges

CH 431 Physical Chemistry
Hangzhou Study Abroad
Instructor: Dr. Stefan Franzen,
Email: Stefan_Franzen@ncsu.edu
Text: Physical Chemistry, Atkins and DePaula, 8th Edition, Oxford University Press

Course goals: To present an introduction to essentials of physical chemistry and to outline the general physical principles that form the basic framework for Chemists with applications to other branches of chemistry ranging from biochemistry and engineering. The course emphasis will be given to molecular structure and spectroscopy.

Problem sets: Problem sets will be assigned in class on a regular basis. Problem sets should be turned in after one week they are assigned. Please staple sheets in order with name, date, and assignment identification clearly printed in the upper right corner of the cover page.

Course prerequisites (NCSU courses): CH 201/202; MA 241 or 242, PY 205 or PY 211

Recitation: You must sign up for a 50 min problem session. There will be two problem sessions offered each week. While no separate grade is assigned for CH 431P, any graded quizzes given there will count towards your grade in CH 431.

Other policies: Talking is prohibited during lectures. Excessive shuffling while lecture is in progress is distracting for everyone. **For problem sets and discussions we encourage you to work in groups of two or three**. Test yourself using practice exams without the help of fellow students. Make sure you can work the problems on your own before the exam.

(note: dates are based on 2010 program. 2011 will include an additional week of classes)
Date Main Lecture Topic Reading Second lecture topic
1. May 17 Quantum vs Classical Physics Chapter 8.1-8.2
2. May 18 The wave equation Chapter 8.3-8.7
3. May 19 Particle in a box Chapter 9.1-9.3
4. May 20 Rotational States,
Angular momentum
Chapter 9.4-9.4 Recitation
5. May 21 The Harmonic Oscillator Chapter 9.6-9.8
6. May 24 The Hydrogen Atom Chapter 10.1-10.3
7. May 25 Many-Electron Atoms Chapter 10.4-10.9 Recitation
8. May 26 The variation principle Chapter 11.1
9. May 27 Diatomic molecules Chapter 11.2-11.5 Recitation
10. May 28 Molecular Structure I Chapter 11.6-11.7
11. May 31 Molecular Structure II Chapter 11.8
12. June 1 Ab initio Calculations Recitation
13. June 2 Group Theory Applications Chapter 12.1-12.3
14 June 3 Group Theory Applications Chapter 12.4-12.6 Recitation
15. June 4 Mid-term
16. June 7 Introduction to Spectroscopy Chapter 13.1-13.3
17. June 8 Vibrational Spectroscopy Chapter 13.9-13.13 Recitation
18. June 9 Rotational Spectroscopy Chapter 13.4-13.8
19. June 10 Electronic spectroscopy Chapter 14.1-14.2 Recitation
20. June 11 Fluorescence, Stimulated Emission Chapter 14.3
21. June 14 Lasers and applications Chapter 14.514.6
22. June 15 Rayleigh and Raman Scattering Recitation

23. June 16 NMR Spectroscopy Chapter 15.1-15.7
24. June 17 Vector and Product Operator Chapter 15.8-15.13 Recitation
25. June 18 X-ray crystallography Chapter 20.1-20.3
26. June 21 Statistical Thermodynamics Chapter 16.1-16.2
27. June 22 Statistical Thermodynamics Chapter 16.3-16.7 Recitation
28. June 23 Molecular Dynamics Chapter 17.1-17.2
29. June 24 System Properties Chapter 17.3-17.8 Recitation
30. June 25 Review
31. June 28 Final Exam

Grades will be based as follows: There will be +/- grading.
Quizzes and Homework 300 pts
Mid-Terms 400 pts
Final Exam 300 pts
Semester Total 1000 pts

Physical Chemistry
CH 433, Summer 2010
Professor: Dr. Stefan Franzen
E-mail: Stefan_Franzen@ncsu.edu

Course goals: To present an introduction to essentials of physical chemistry and to outline the general physical principles that form the basic framework for Chemists with applications to other branches of chemistry ranging from biochemistry and engineering. The course emphasis will be given to thermodynamics and kinetics. Textbook: "Physical Chemistry", by Atkins and DePaula, 8th Edition, Oxford University Press Problem sets: Problem sets will be assigned in class on a regular basis. Problem sets should be turned in after one week they are assigned. Please staple sheets in order with name, date, and assignment identification clearly printed in the upper right corner of the cover page.
Incomplete grades and late assignments: If a student is granted with a reasonable documented excused absence according to the University policy, then the grades for the missed assignment(s) will be determined as follows: either an alternative (make-up) exam or assignment will be given and/or the total maximum of the points for the student will be decreased by the points corresponding to the missed assignment(s) and the new (decreased) number of the maximum points be used to renormalize the number of the points earned. If no reasonable excuses are given the student will not be credited with any points for the missed assignment and the total maximum number of points will not be re-normalized. **Excuses for any anticipated exam absence** must be presented no later than **one week** prior to the exam. The only exception to this policy is for documented medical emergencies.

Course prerequisites(NCSU courses): CH 201/202; MA 241 or 242, PY 205 or PY 211
Recitation: You must sign up for a 50 min problem session. There will be two problem sessions offered each week. While no separate grade is assigned for CH 431P, any graded quizzes given there will count towards your grade in CH 431.
Academic integrity: All exams and quizzes are expected to be completed in accordance with the Code of Student Conduct adopted by the University. It is my understanding and expectation that the student's signature on any test means that the student neither gave nor received unauthorized aid.
Students with disabilities: Students with disabilities will be accommodated according to the University policy.

Other policies: Talking is prohibited during lectures. Excessive shuffling while lecture is in progress is distracting for everyone. **For problem sets and discussions we encourage you to work in groups of two or three.** Test yourself using practice exams without the help of fellow students. Make sure you can work the problems on your own before the exam.

Date Main Lecture Topic Reading Recitation Schedule
1. May 20 Macroscopic vs. Microscopic Chapter 1.1-1.3
2. May 21 Properties of Gases Chapter 1.4
3. May 24 Real Gases/Corresponding States Chapter 1.5 Recitation
4. May 25 The First Law Chapter 2.1-2.3
5. May 26 Enthalpy, Heat Capacity Chapter 2.4-2.9 Recitation
6. May 27 Entropy and the 2nd Law Change 3.1-3.3
7. May 28 Second Law Applications
8. May 31 Entropy and the Third Law Chapter 3.4
9. June 1 Gibbs Free Energy Chapter 3.5-3.6 Recitation
10. June 2 Free energy applications Chapter 7.1-7.2
11 June 3 The Clausius-Clapeyron Eqn. Chapter 4.1-4.3 Recitation
12. June 4 Phase Equilibria Chapter 4.4-4.7
13. June 7 Colligative Properties Chapter 7.3.7.4 Recitation
14. June 8 Mid-term

15. June 9 Maxwell Relations Chapter 3.7-3.9 Recitation
16. June 10 Solutions – Real and Ideal Chapter 5
17. June 11 Gibbs-Duhem
18. June 14 Phase Diagrams Chapter 6 Recitation
19. June 15 Transport properties Chapter 19
Chapter 21.9-21.10
20. June 16 Introduction to Kinetics Chapter 22.1-22.5 Recitation
21. June 17 Rate Laws Chapte3 22.6-22.8
22. June 18 Complex reactions Chapter 23
23. June 21 Arrhenius Equation Chapter 24.1-24.5 Recitation
24. June 22 Transition State Theory Chapter 24.6-24.9
25. June 23 Reaction dynamics Chapter 24.10-24.12
Recitation
26. June 24 Catalysts/Surfaces Chapter 25
27. June 25 Review
28. June 28 Final Exam
Grades will be based as follows: There will be +/- grading.
Quizzes and Homework 300 pts
Mid-Terms 400 pts
Final Exam 300 pts
Semester Total 1000 pts

CH 499 **Research Overview**

The research component of this program is designed to meet the need of technical students who have a laboratory, research or capstone requirement. For practical reasons we will emphasize computational projects, but this is not a requirement. There are opportunities for laboratory experiences that can be discussed individually with the Director.

Computational projects involve the use of molecular dynamics or quantum chemistry to solve problems of interest to research groups at Zhejiang University. Since these groups collaborate with the Director there are components that will be initiated at NCSU. This is an integrated program that will involve preparation at NCSU followed by intensive work with Zhejiang University graduate students and professors. The level of expertise that the students will experience is extremely high. This is a unique opportunity to work closely with expert researchers. Chinese graduate students are anxious to meet U.S. students. Nowadays, the level of English language spoken is very high. There will not be a problem with communication. The Director will emphasize to the Chinese students the value of instructing the U.S. students in Chinese as a component of the program. This is a great way for them to improve their English while helping U.S. students acclimate. While there is no language requirement for this program, there will be ample opportunity for interested students to learn rudimentary Chinese in a unique method. The Director speaks Chinese and will also provide basic instruction in "Survival Chinese". Students can learn either molecular dynamics (MD) or the quantum chemical method, density functional theory (DFT). The code used is freeware so that students will be able to use the skills gained in any computational environment, once they have learned the basics.

The MD code used is VMD/NAMD written and distributed by the Schulten group at the University of Illinois. VMD is a GUI interface that is easy to use and provides a powerful way to visualize proteins, DNA etc. NAMD stands for "Not Another Molecular Dynamics" code. Prof. Schulten has a sense of humor. His code is the fastest code written and runs very well on parallel environments. However, it can also run on a PC (just a little slowly).

The DFT code used is ORCA written and distributed by the Neese group at the University of Bonn. ORCA has become a versatile code that can be used for structure and spectroscopy. It currently has over 3000 users worldwide. ORCA is widely used for the study of metal centers in catalysis, which will be our main application.

Research topics include (but are not limited to)
MD studies of receptor-binding in cell targeting studies.
MD studies of dynamics and mutational analysis of dehaloperoxidase and related enzymes.
DFT studies of oxidative metal enzymes and industrial oxidation catalysts.