

Center for Workshops in the Chemical Sciences, CWCS, workshop:

Theoretical and Computational Chemistry

May 15 – May 20, 2005 Salt Lake City, Utah

Workshop Objective

Expose participants to modern theoretical and computational tools to understand fundamental chemistry problems. This includes electronic structure, and nuclear motion in describing gas-phase as well as condensed-phase stationary and time-dependent phenomena.

General Contact Information

Accommodations: Homestead Studio Suites
1220 E. 2100 S.
Salt Lake City, UT 84106
Telephone: 801-474-0771

Reimbursement Contact: Cary Lyle
Department of Chemistry
P.O. Box 4098
Georgia State University
Atlanta, GA 30302-4098
cary-lyle@gsu.edu

Workshop Instructors

- **Rigoberto Hernandez**
Associate Professor
School of Chemistry and Biochemistry
Georgia Institute of Technology
E-mail: hernandez@chemistry.gatech.edu
- **David Sherrill**
Associate Professor
School of Chemistry and Biochemistry
Georgia Institute of Technology
E-mail: sherrill@chemistry.gatech.edu
- **Tricia Shepherd**
Assistant Professor
Westminster College
E-mail: tshpherd@westminstercollege.edu

Guest Speaker

Jack Simons
Professor
Department of Chemistry
University of Utah
E-mail: simons@chem.utah.edu

General Schedule

SUNDAY WELCOMING RECEPTION

- 6:00-6:15 pm: Meet in lobby of hotel for shuttle transportation to Westminster College (We will be using Westminster College vans to transport participants to the college, or you can make your own arrangements for transportation.)
- 6:15-7:00 pm: Appetizers, Introductions (Jewett Center – EEJC Tanner Atrium)
- 7:00-9:00 pm: Dinner (Jewett Center – EEJC Tanner Atrium)

WORKSHOP SCHEDULE MON-FRI

- *Breakfast:* (on your own)
- 8:30: Depart for Westminster College – Use college shuttle van -or- car-pool -or- shared taxi (taxi will be reimbursed) -or- walk
- 9:00-12:15: *Lectures:* Gore 206
- 12:15-1:30: *Lunch:* Shaw Student Center
- 1:30-4:30: *Computer Laboratory:* Malouf 203
- 4:30: Depart for hotel (college shuttle van)
- *Dinner:* (on your own – except for Monday night reception)

MONDAY RECEPTION

- 5:45-6:00 pm: Meet in Lobby of Hotel for Shuttle Transportation to Westminster
- 6:00-8:00 pm: Dinner (Giovale Library – Watson Board Room) with guest speaker

FRIDAY

Workshop ends at noon. Check -out of hotel in morning, check baggage at hotel or bring to morning session

Accommodations

Homestead Studio Suites, 1220 E. 2100 S, Salt Lake City, 84106 (ph: 801-474-0771).
Lodging expenses (room only) are direct billed to CWCS program
Participants will be responsible for incidentals charged at hotel

Directions to Hotel:

--From I-80 West, go to 1300 East/Sugar House. Exit #126. Turn right at the traffic signal. Drive ½ mile north to 2100 South. Turn left. Drive 1/10 of a mile west and look for Homestead on the left.

--From Salt Lake International Airport, Take Bangerter highway South for approximately 3 miles to State Road 201 East. Turn left on SR 201. Drive east on SR 201 for approximately 4 miles to I-80 East. Exit onto I-80 East (Cheyenne exit). Drive east on I-80 for approximately 3 miles to 1300 East/Sugar House exit #126. Turn left at traffic signal. Drive north ½ mile to 2100 South. Turn left at the traffic signal. Drive west 1/10 mile and look for Homestead on the left.

Emergency contact information

--If somebody needs to contact you during the workshop they may contact the hotel (801-474-0771), or Pam Cote (801-832-2304; pcote@westminstercollege.edu).

Accounting

NOTE: all claims for reimbursement require original receipts (please attach receipts to 8.5 x 11 paper and submit with request form)

Reimbursable expenses:

- Up to \$32 per day meal expenses
- Shared taxi

Send all requests for reimbursement to Cary Lyle at GSU.

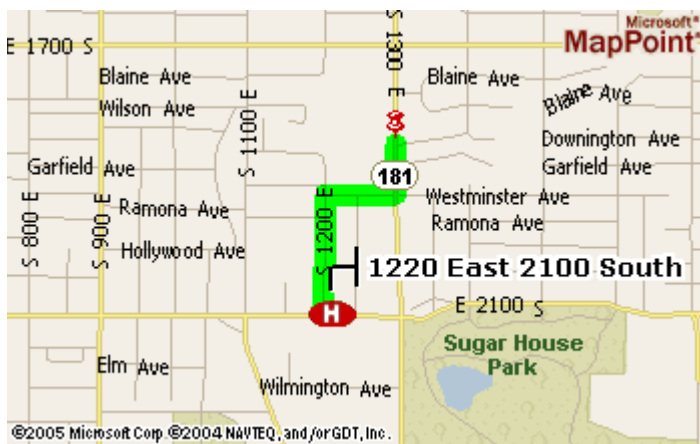
Cary Lyle
Department of Chemistry
P.O. Box 4098
Georgia State University
Atlanta, GA 30302-4098
cary-lyle@gsu.edu

Requests should include form

(http://chemistry.gsu.edu/CWCS/Food_Reimbursemen_Form.pdf) and must include SSN.

Directions

From the hotel, go north on 1200 E to Westminster Ave. Turn Right (East) go one block to 1300 E. Turn Left (North) go one block to Westminster College. Visitor Parking spaces are available in the parking area adjacent to 1300 East and Foster Hall.



Westminster Campus Map

Westminster College
1840 South 1300 East
Salt Lake City, Utah 84105



1. Converse Hall
2. Bill and Vieve Gore School of Business
3. Giovale Library
4. Malouf Hall and Dick Science Building
5. Olwell Hall
6. Behnken Hall
7. Stock Hall
8. Shaw Student Center
9. Payne Gymnasium
10. Jewett Center for the Performing Arts
11. Nightingale Hall
12. Foster Hall
13. Dolores Dore Eccles Ceramic Center
14. Nunemaker Place
15. Carleson Hall
16. Communication Office
17. Bamberger Hall
18. Hogle Hall
19. Walker Hall

Detailed Daily Schedule

Sunday, May 15: Check-in to hotel

- 6:00pm – Depart for Westminster College (shuttle van)
- 6:15pm – Welcoming Reception/Dinner (Tanner Atrium, Jewett Center)

Monday, May 16: Day one

- 8:30am – Depart for Westminster (shuttle van)
- 9:00am – Lecture 1: Molecular Mechanics: Sherrill
- 10:30am – Break
- 10:45am – Lecture 2: Hartree-Fock Molecular Orbital Theory: Sherrill
- 12:15pm – Lunch
- 1:30pm – Lab 1: Molecular Mechanics: Shepherd
- 4:30pm – Depart for hotel (shuttle van)
- 5:45pm – Depart for Westminster College (shuttle van)
- 6:00pm – Dinner (Watson Board Room, Giovale Library) Guest Speaker: Professor Jack Simons, University of Utah

Tuesday, May 17: Day two

- 8:30am – Depart for Westminster (shuttle van)
- 9:00am – Lecture 3: Electron Correlation Methods: Sherrill
- 10:30am – Break
- 10:45am – Lecture 4: Geometry Optimization: Sherrill
- 12:15pm – Lunch
- 1:30pm – Lab 2: Electronic Structure: Shepherd
- 4:30pm – Depart for hotel (shuttle van)

Wednesday, May 18: Day three

- 8:30am – Depart for Westminster (shuttle van)
- 9:00am – Lecture 5: Research Presentation: Sherrill
- 10:30am – Break
- 10:45am – Lecture 6: Review of Classical Mechanics: Hernandez
- 12:15pm – Lunch
- 1:30pm – Lab 3: Ising Model: Shepherd
- 4:30pm – Depart for hotel (shuttle van)

Thursday, May 19: Day four

- 8:30am – Depart for Westminster (shuttle van)
- 9:00am – Lecture 7: Statistical Mechanics, Ideal Systems: Hernandez
- 10:30am – Break
- 10:45am – Lecture 8: Nonideal Systems, Spin Ising Model: Hernandez
- 12:15pm – Lunch
- 1:30pm – Lab 4: Liquid Structure: Shepherd
- 4:30pm – Depart for hotel (shuttle van)

Friday, May 20: Day five

- 8:30am – Depart for Westminster (shuttle van)
- 9:00am – Lecture 9: Continuum Liquids: Hernandez
- 10:30am – Break
- 10:45am – Lecture 10: Research Presentation: Hernandez

Workshop Materials and Handouts

Note: You will be given paper versions of all handouts at the workshop, including preliminary handouts e-mailed in advance.

Lecture

- Introduction to Electronic Structure Theory
- The Born-Oppenheimer Approximation
- Molecular Mechanics
- Introduction to Hartree-Fock Molecular Orbital Theory
- Basis Sets in Quantum Chemistry
- Introduction to Electron Correlation
- Geometry Optimization
- Molecular Vibrations
- Computing Thermodynamic Quantities

Lab

- UNIX Basics
- vi Editor Basics
- Programming Basics - FORTRAN 77
- The Center for Computational Molecular Science and Technology
- Spartan Tutorial
- Lab 1: Molecular Mechanics
- Lab 2: Electronic Structure
- Lab 3: Ising Model
- Lab 4: Liquid Structure

Molecular Modelling: Principles and Applications

by [Andrew R. Leach](#)

Articles from the *Journal of Chemical Education* highlighting the use of computational chemistry in the undergraduate curriculum