

# Chemistry 450 / 750

## Atomic & Molecular Clusters

Lectures: 19:00 – 22:00 Th  
Course Instructor: Dr. Scott Hopkins

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Atomic and molecular clusters constitute intermediates between molecules, with clearly defined quantum states, and condensed matter where these states form bands or continua. As such, the study of clusters can be viewed as a means of unravelling the evolution of bulk properties from those of the constituent atoms/molecules. Interestingly, owing to the high ratio of surface atoms to bulk atoms, there are many analogies between the chemistry and physics of clusters and of solid surfaces. For this reason, clusters have traditionally been regarded as test cases for the study of surface reactivity and heterogeneous catalytic activity. More recently, however, attention has shifted towards cluster finite size effects, which lead to electronic, magnetic, optical, and chemical properties that are quite different from those of molecules or condensed matter. Now, the use of clusters as components in nanodevices is also attracting a great deal of attention. This course will describe the experimental generation, detection and interrogation of clusters, as well as the theoretical approaches that have been developed to aid in our understanding of their physical properties.

Chemistry 450/750 will be managed using the Desire2Learn (D2L) learning management system, which can be accessed via the LEARN facility at <https://learn.uwaterloo.ca>. This site will provide course information, problem set postings and solutions, schedules, supplementary lecture material, practise quizzes, and other information that you might find useful. Please subscribe to notifications from the D2L CHEM 450/750 page.

The text for this course is a comprehensive set of notes that will be available on the course site. Students will also find the text “Atomic and Molecular Clusters” by Roy L. Johnston to be useful. This book can be found in the UW Davis library (QC173.4.M48 J64). A second text titled “Atomic and Molecular Clusters” by Elliot R. Bernstein (QD461.A857) is also available to students at UW for further reading. For an in depth study of cluster potential energy surfaces, the text “Energy Landscapes” by David J. Wales (QD462.6.P64 W35) is an excellent resource.

Absences from exams or missed problem sets may be accommodated *only if* a completed Verification of Illness form (available from the “About Us” link at <http://www.healthservices.uwaterloo.ca>) is turned in to the Science Undergraduate Office in ESC-252. Absence for other reasons will result in a grade of **zero** for that component of the coursework.

You are expected to be familiar with the UW expectations of Academic Integrity, and you are encouraged to complete the online quiz at <http://www.lib.uwaterloo.ca/ait/>.

## Course Outline

Unit 1 – Introduction to Cluster Theory

Unit 2 – Cluster Science in Practise

Unit 3 – Case Studies

## Case Study (Chem 750 students only)

Chem 750 will be required to undertake a case study that will constitute 20% of their course mark. The case study will involve a critical analysis of a current topic in atomic and molecular cluster research, which will be assessed with a written report (20 page maximum) and a 30 minute in-class seminar, each worth 10% of the student's overall grade. Several suggested topics are given below, but the student may choose a topic not listed, provided this is first approved by the course instructor.

### Case study topics:

1. "C-H activation of alkanes on  $Rh_n^+$  ( $n = 1-30$ ) clusters: Size effects on dehydrogenation", Adlhart, C. and Uggerud, E., *J. Chem. Phys.*, **123**, 214709 (2005)
2. "Amyloid- $\beta$  protein oligomerization and the importance of tetramers and dodecamers in the aetiology of Alzheimer's disease", Bernstein, S. L., *et al.*, *Nature Chemistry*, **1**, 326 (2009)
3. "Electric deflection studies of rhodium clusters", Beyer, M. K., and Knickelbein, M. B., *J. Chem. Phys.*, **126**, 104301 (2007)
4. "Clusters, Superatoms, and Building Blocks of New Materials", Castleman, Jr., A. W., and Khanna, S. N., *J. Phys. Chem. C*, **113**, 2664 (2009)
5. "Structures of Neutral  $Au_7$ ,  $Au_{19}$  and  $Au_{20}$  Clusters in the Gas Phase", Gruene, P., *et al.*, *Science*, **321**, 674 (2008)
6. "Structure determination of neutral Mg clusters – hexagonal nanotubes and cages", Haertelt, M., *et al.*, *Phys. Chem. Chem. Phys.*, **14**, 2849 (2012)
7. "Global minima of protonated water clusters", Hodges, M. P., and Wales, D. J., *Chem. Phys. Lett.*, **324**, 279 (2000)
8. "Infrared photodissociation spectroscopy of  $H^+(H_2O)_6 \bullet M_m$  ( $M = Ne, Ar, Kr, Xe, H_2, N_2$  and  $CH_4$ ): messenger-dependent balance between  $H_3O^+$  and  $H_5O_2^+$  core isomers", Mizuse, K., and Fujii, A., *Phys. Chem. Chem. Phys.*, **13**, 7129 (2011)
9. "Electronic and geometric properties of exohedral sodium- and gold-fullerenes", Palpant, B., *et al.*, *J. Chem. Phys.*, **114**, 8459 (2001)
10. "Aromatic Metal-Centered Monocyclic Boron Rings:  $Co@B_8^-$  and  $Ru@B_9^-$ ", Romanescu, C., *et al.*, *Angew. Chem. Int. Ed.*, **50**, 9334 (2011)

11. "Quantum Solvation of Carbonyl Sulfide with Helium Atoms", Tang, J., *et al.*, *Science*, **297**, 2030, (2002)
12. "Observation of Large Water-Cluster Anions with Surface-Bound Excess Electrons", Verlet, J. R. R., *et al.*, *Science*, **307**, 93 (2005)
13. "Infrared photodissociation spectroscopy of  $V^+(CO_2)_n$  and  $V^+(CO_2)_nAr$  complexes", Walker, N. R., *et al.*, *J. Chem. Phys.*, **120**, 10037 (2004)
14. "The Structure of Protonated Water Clusters", Zwier, T. S., *Science*, **304**, 1119 (2004)

## Grades

### Chem 450

**Assignments:** 10 – 15 % (5 at roughly bi-weekly intervals)

**Mid-term Exams:** 10 – 15 % (two of; to be scheduled)

**Final Exam:** 55 – 70 % (to be scheduled)

### Chem 750

**Assignments:** 10 % (5 at roughly bi-weekly intervals)

**Mid-term Exams:** 10% (two of; to be scheduled)

**Case Study:** 20% (10% written report, 10% seminar)

**Final Exam:** 60% (to be scheduled)

## Statement for students with disabilities

Note for students with disabilities: The Office for Persons with Disabilities (OPD), located in Needles Hall, Room 1132, collaborates with all academic departments to arrange appropriate accommodations for students with disabilities without compromising the academic integrity of the curriculum. If you require academic accommodations to lessen the impact of your disability, please register with the OPD at the beginning of each academic term.

## Statement regarding travel and the final examination period

Student travel plans are not considered acceptable grounds for granting an alternative examination time (see <http://www.registrar.uwaterloo.ca/exams/finalexams.html>). The final exam schedule is usually posted about 5 or 6 weeks into the term, so start checking towards the end of February.

## Expectation of academic integrity

**Academic Integrity:** *In order to maintain a culture of academic integrity, members of the University of Waterloo community are expected to promote honesty, trust, fairness, respect and responsibility.*

**Grievance:** *A student who believes that a decision affecting some aspect of his/her university life has been unfair or unreasonable may have grounds for initiating a grievance. Read Policy #70, Student Petitions and Grievances, Section 4. <http://www.adm.uwaterloo.ca/infosec/Policies/policy70.htm>*

**Discipline:** *A student is expected to know what constitutes academic integrity, to avoid committing academic offenses, and to take responsibility for his/her actions. A student who is unsure whether an action constitutes an offense, or who needs help in learning how to avoid offenses (e.g., plagiarism, cheating) or about “rules” for group work/collaboration should seek guidance from the course professor, academic advisor, or the Undergraduate Associate Dean. For information on categories of offenses and types of penalties, students should refer to Policy #71, Student Discipline, <http://www.adm.uwaterloo.ca/infosec/Policies/policy71.htm>*

**Appeals:** *Concerning a decision made under Policy #70 (Student Petitions and Grievances) (other than petitions) or Policy #71 (Student Discipline) a student may appeal the finding, the penalty, or both. A student who believes he/she has a ground for an appeal should refer to Policy #72 (Student Appeals) <http://www.adm.uwaterloo.ca/infosec/Policies/policy72.htm>*