Course: CHMC20H3F, Intermediate Physical Chemistry

Instructor: Prof. Artur F. Izmaylov, **e-mail:** aizmaylov@utsc.utoronto.ca

TA: TBA, **e-mail:** TBA

Please use only UofT email accounts. When composing your email, please use professional language. Be sure to include the course code as part of the subject line and sign the email with your first and last name, as well as your student ID. Your email will be answered as soon as possible.

Web: CHMC20 maintains a Quercus web space which archives a variety of course-related information including: grades, class announcements, lecture and lab materials, contact information and links to outside resources. In addition, class emails will periodically be sent via Quercus. To receive these emails, you must have a valid "utoronto.ca" email account registered with ROSI.

Office: EV356; office hours: Wednesday 14:00–15:30

Lectures: Room AA 205, Wednesday 12:00–14:00

Recommended Texts: 1) Ira Levine, Physical Chemistry; 2) Atkins and de Paula, Physical Chemistry, 3) D. A. McQuarrie, Statistical Mechanics; 4) A. Szabo and N.S. Ostlund, Modern quantum chemistry: Introduction to advanced electronic structure theory

Marking Scheme: midterm test 35%, final exam 45%, homeworks 20%: will appear on Wednesdays (starting Sept 11, check Quercus), will be due noon of the next Wednesday, -50% late penalty.

Note: To pass this course you need to pass either the midterm test or the final exam, visit me during the office hours at least once before the midterm test, and receive a final grade of 50+.

Course Description: This course gives an introduction to statistical mechanics and electronic structure. These subjects will be applied to thermochemistry, kinetics, and spectroscopy. The list of topics is as follows.

•Motivation for statistical mechanics, elements of probability theory

•Ensembles in statistical mechanics: micro-canonical, canonical, and grand-canonical ensembles

•Relation between statistical mechanics and thermodynamics

•Partition function for molecular systems (translational, rotational, vibrational, and electronic components), chemical equilibrium

•Electronic structure, Hartree-Fock method, molecular geometry, harmonic frequencies

Midterm:

There will be a take-home mid-term test on Oct 23rd. If you miss the mid-term due to a legitimate reason, you must submit appropriate documentation *within one week of your absence.* If the reason is medical, an official UTSC medical form should be downloaded from the Registrar's website http://www.utsc.utoronto.ca/~registrar/resources/pdf_general/UTSCmedicalcertificate.pdf and completed by your physician. Students with a validated absence will be permitted to write a make-up exam. ***If no acceptable documentation is received, you will receive a grade of zero for that test.***

Final Examination:

There will be a 3-hour, ***cumulative*** exam written during the end of semester exam period. The exact date, time and location will be announced as soon as they are available.
Please note that if you miss the Final Exam, you must petition the Registrar's Office to write a make-up exam in the next formal exam period. e.g. for a missed April Final Exam, the make-up Exam is in August. Your documentation is crucial for a successful petition and must be submitted by the last day of the exam period. Check the UTSC Calendar for instructions and deadlines.

On Academic Integrity:

Academic integrity is essential to the pursuit of learning and scholarship in a university, and to ensuring that a degree from the University of Toronto is a strong signal of each student's individual academic achievement. As a result, the University treats cases of cheating and plagiarism very seriously. The University of Toronto's Code of Behaviour on Academic Matters (www.governingcouncil.utoronto.ca/policies/behaveac.htm) outlines the behaviours that constitute academic dishonesty and the processes for addressing academic offences. Potential offences include, but are not limited to:

In papers and assignments:

1. Using someone else's ideas or words without appropriate acknowledgement.
2. Submitting your own work in more than one course without the permission of the instructor.
3. Making up sources or facts.
4. Obtaining or providing unauthorized assistance on any assignment.

On tests and exams:

1. Using or possessing unauthorized aids.
2. Looking at someone else's answers during an exam or test.

3. Misrepresenting your identity.

In academic work:

1. Falsifying institutional documents or grades.
2. Falsifying or altering any documentation required by the University, including (but not limited to) doctor's notes.

All suspected cases of academic dishonesty will be investigated following procedures outlined in the Code of Behaviour on Academic Matters. If you have questions or concerns about what constitutes appropriate academic behaviour or appropriate research and citation methods, you are expected to seek out additional information on academic integrity from your instructor or from other institutional resources (see **www.utoronto.ca/academicintegrity/resourcesforstudents.html**).

On Accommodation:

The University provides academic accommodations for students with disabilities in accordance with the terms of the Ontario Human Rights Code. This occurs through a collaborative process that acknowledges a collective obligation to develop an accessible learning environment that both meets the needs of students and preserves the essential academic requirements of the University's courses and programs.

For more information on services and resources available to instructors and students, please contact Tanya Lewis, Director, Academic Skills and Accessibility Services at 416-978-6786; **tanya.lewis@utoronto.ca**.