UNIVERSITY OF CALGARY
FACULTY OF SCIENCE
DEPARTMENT OF CHEMISTRY
COURSE SYLLABUS
WINTER 2020

1. Course: Course ID and number, Course Title (e.g. **CHEMISTRY 689.11,** Selected Topics in Physical Chemistry (**Heterogeneous Catalysis**)
)

LEC	DAYS	TIME	ROOM	INSTRUCTOR	OFFICE	EMAIL	OFFICE HOURS
L01	Tue/ Thurs	14:00-15:15	SA 249	Dr. S. Siahrostami	EEEL 507	samira.siahrostami@ucalgary.ca	Tue 10-12 am

Course Desire 2 Learn (D2L) Chem 689.11, Selected Topics in Physical Chemistry, Heterogenous Catalysis

Department of Chemistry: Room SA 229, Tel: (403) 220-5341, e-mail: chem.info@ucalgary.ca

Students must use their U of C account for all course correspondence.

2. Course Description: The course focuses on atomic scale understanding of heterogenous catalysis and gives an overview of modelling reactions at the catalyst surfaces.

3. Grading: The University policy on grading and related matters is described sections F.1 and F.2 of the online University Calendar. In determining the overall grade in the course the following weights will be used:

Assignments (8)	20%
Midterm seminars	40%
Final Project	40%

Each piece of work (reports, assignments, quizzes, midterm exam(s) or final examination) submitted by the student will be assigned a grade. The student's grade for each component listed above will be combined with the indicated weights to produce an overall percentage for the course, which will be used to determine the course letter grade.

The conversion between a percentage grade and letter grade is as follows: **(Example)**

A+	A	A-	B+	B	B-
95% - 100%	87% - 94%	82% - 86%	77% - 81%	72% -76%	66% - 71%

C+	C	C-	D+	D	F
62% - 65%	58% - 61%	54% - 57%	50% - 53%	45% - 49%	< 44%

4. Missed Components of Term Work: There are no deferred Midterm/ term test examinations

In the event that a student misses the midterm or any course work due to illness, supporting documentation, such as a medical note or a statutory declaration will be required (see Section N.1; for more information regarding the use of statuary declaration/ medical notes, see FAQ). Absences must be reported **within 48 hrs**.

The regulations of the Faculty of Science pertaining to this matter are found in the Faculty of Science area of the Calendar in Section 3.6. It is the student's responsibility to familiarize himself/herself with these regulations. See also Section E.3 of the University Calendar.

If a student misses the midterm for other reasons, then analogous documentation will be required. The course coordinator will need to see the original documentation (not electronic copy) for review / decision and keep it (or a copy) for their records. The documentation must be provided to the course coordinator **within 15 days** of the date of the midterm in order for an excused absence to be considered. If an excused absence is approved, then the percentage weight of a legitimately missed midterm examination *will be pro-rated among the remaining components*

of the course OR will be transferred to the final examination (see Section E.3 of the University Calendar) [Choose one of these two options].

If a student missed an experiment or a make-up lab for non-legitimate reasons (e.g. vacation, incomplete or insufficient score in pre-lab assignment), and did not perform the experiment, the contribution of that experiment in the final course grade will be zero.

5. **Course Materials:** 1- Nørskov, Studt, Abild-Pedersen, Bligaard, Fundamental Concepts in Heterogeneous Catalysis, Wiley, 2014. 2- Sholl, Steckel, Density Functional Theory, A Practical Introduction, Wiley 2009.

6. **Topics Covered**:

1. Heterogenous Catalysis and a Sustainable Future
2. The potential Energy Diagram
3. Surface Equilibria
4. Rate Constant and Kinetics
5. Energy Trends in Catalysis
6. Electronic Factor in Heterogenous Catalysis
7. Catalyst structure: Nature of the Active Sites
8. Poisoning and Promotion of Catalysts
9. Surface Electrocatalysis
10. Machine learning in Catalysis

The following signature lines should be added to the course outline <u>as appropriate</u>

Department Approval_____Electronically Approved_____Date_____January 6, 2020_____