UNIVERSITY OF CALGARY
FACULTY OF SCIENCE
DEPARTMENT OF CHEMISTRY
COURSE SYLLABUS
FALL 2017

1. **Course: CHEMISTRY 659.21, Advances in Organic Materials**
   Lecture Sections: L01
   MWF, 9-9:50, SA 123, Dr. Sutherland (SB220, 403.220.7559 sutherlt@ucalgary.ca)
   Office Hours: by appointment

   Chemistry Departmental Office Science A 229, 403.220.5341, chem.undergrad@ucalgary.ca

   To avoid IT problems, it is recommended that the students use their U of C account for all course correspondence.

   Desire 2 Learn (D2L): CHEM 659.21 L01 - (Fall 2017) - Advances in Organic Materials
   https://d2l.ucalgary.ca/

2. **Course Description:** ***Lectures:*** We will discuss the operating principles of small molecule organic electronic devices, including field-effect transistors, photovoltaics and light-emitting diodes. Next, we will examine critically modern examples of high performance materials stressing the relationship between molecular properties and materials design. Many of the physical techniques used, such as photochemistry and electrochemistry, will be explored through assignments to achieve quantifiable assessments.

Chem 659.21 Advances in Organic Materials

Classes will be held MWF at 9-9:50, SA 123in SA 123.

The semester Schedule will be built once enrollment has been finalized, but the following important due dates are fixed:

Assignments: 1 - due 29 September; 2 - due 13 October; 3 – due 6 November.

Term papers: 1: due 8 November; 2 – due 11 December.

Assignments: All assignments will be given a numerical grade from 0 to 10 and late reports will be deducted 2.5 marks per day. Following the due date, a group of students indicated in the schedule will 'teach' the class how they arrived at their answers. All assignment will total 20% of your final grade.

Presentations: *Papers:* The indicated student will present a paper, relevant background (15 minutes) followed by discussion for the remainder of the class. The indicated student will email the paper to the class one week prior to the talk and each student (except presenter) will email the instructor three questions by noon one day prior to the talk.

Assignments: The indicated group of students will present their approach to answering the assignment questions in a teaching format to the class (1 lecture).

Proposals: there will be a midterm proposal presentation where each indicated student will pitch their proposal ideas for 20 minutes using this opportunity for feedback to enhance their written proposal. Each student will get a second chance to improve their proposal pitch of their refined presentation at the end of the semester.

All presentations will total 20% of your final grade.

Term papers: Two term papers are required for this course and the details are below. You will receive a grade from 0 to 10 for each paper and late reports are subjected to 2.5 marks per day penalty. All term papers will total 60% of your final grade.

CHEM 659.21 – Assignment 1, due Sept 29th, 9am.

Using the data in the attached data file 'Assignment1-Data.xlsl' please calculate the oscillator strength of the lowest energy transition using Excel's curve fitting 'solver' as demonstrated in lecture. Assume the peak(s) are Gaussian-shaped. You will need to find the definition of oscillator strength and how it is determined and a general equation of a Gaussian shape would help. The included data are absorption spectra for three different pyrene isomers from our lab in x,y data pairs of wavelength in nanometers and absorbance.

1) I need to see each raw data plotted appropriately, overlayed with a line of the best fit and a plot of residuals (difference between observed and fit data) for all three compounds. Please submit the Excel file as part of your answer.

2) Include a narrative of the steps involved in getting the answers with appropriate references.

CHEM 659.21 – Assignment 2, due October 13th 9am.

Using the data in the attached data file 'Assignment2-Data.xlsl' please calculate the HOMO-LUMO energy gap in eV and the E_{HOMO} and E_{LUMO} versus vacuum.

1) I need to see each raw data plotted appropriately and how each parameter was measure from the plots. Please submit the Excel file as part of your answer.

2) Include a narrative of the steps involved in getting the answers with appropriate references.

CHEM 659.21 – Assignment 3, due November 6th 9am.

Using the data in the attached data file 'Assignment3-Data.xlsl' please calculate the monomer to dimer ratio of a chromophore at various concentrations. The monomer has an absorption peak at 500 nm, whereas the dimer has an absorption peak at ~472 nm. Determine the concentration of mono and dimer at each step in the dilution experiment assuming the dimer molar absorptivity is 120,000 $M^{-1}\cdot cm^{-1}$ and the monomer absorptivity is 60 000 $M^{-1}\cdot cm^{-1}$.

1) You will need to carry out peak deconvolution like assignment 1 to assess the concentrations. Include raw data, fit lines and residuals for each concentration. Please submit the Excel file as part of your answer.

2) Include a narrative of the steps involved in getting the answers with appropriate references.

Term paper 1: Critical review, due: Nov. 8 at 9am.

Each of you will write a critical review of the following paper: DOI: 10.1039/c3sc51622a.

A critical review summarizes and evaluates a series of journal articles. Writing a critical review requires you to read the papers in detail and read other related papers (who is citing this work and what are they doing?) so you can present a fair and reasonable evaluation. Being critical does not mean to criticize in a negative manner; rather it requires you to question the information in a paper and present your evaluation. Evaluation is the process that you decide the strengths and weaknesses of the papers. Evaluating requires an understanding of not only the content of the papers, but also an understanding of a paper's purpose. Analyzing requires separating the content and concepts of text into their main components and then understanding how these interrelate, connect and possibly influence each other. The critical review should be broken in the following sections: Introduction, Summary, Critique, Conclusion and References. The bulk of the content should be in the Critique sections (70%). This outline was adapted from http://www.lc.unsw.edu.au/onlib/critrev.html

Requirements:

- 20 pages maximum: double line-spacing- All figures, tables, schemes, etc. must be within text.
- margins: 0.75 inch all around
- 12 pt Times New Roman font
- Follow ACS style guide for tables, figures and referencing format.

Term paper 2 – NSERC proposal, due: Dec. 11 at 9am.

Assignment 2 is to write an NSERC Discovery Grant proposal. For this assignment, assume you just completed a post-doc and you are starting your first faculty position. Build on examples discussed in class and your own experience this far in graduate school and propose a research program. The program should be for 3 graduate students and 3 summer students and span 5 years. In the proposal, identify projects that students will work on, what experiments will be performed, how the data will be anaylsed and expected outcomes. In addition, identify potential pitfalls and back-up plans if project(s) do not work as expected. The following guide is taken from the instructions for professors section of www.nserc.ca. Be creative and innovative in the projects.

PROPOSAL – Total 5 + 2 pages

Using the headings below in 5-pages of single-spaced text (12 pts, Times new Roman, ¾" margins), describe the research to be supported.

- objectives: both short and long term
- literature pertinent to the proposal
- methods and proposed approach
- anticipated impact of the work

Two additional pages are given for references.