

UNIVERSITY OF CALGARY  
FACULTY OF SCIENCE  
DEPARTMENT OF CHEMISTRY  
COURSE SYLLABUS  
FALL - 2019

**Course:** CHEMISTRY 402.01, Introduction Research in Chemistry I

Instructor: Individual Supervisor

**Coordinator:** Dr. Gregory C. Welch, [gregory.welch@ucalgary.ca](mailto:gregory.welch@ucalgary.ca), EEEL 546, 403-210-7603

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 402  
<https://d2l.ucalgary.ca/d2l/home/171384>

Departmental Office: Room SA 229, Tel: (403) 220-5341, e-mail: [chem.undergrad@ucalgary.ca](mailto:chem.undergrad@ucalgary.ca)

Chemistry 402 is a free form course. The faculty supervisor will create a detailed research project outline that includes a breakdown of all grading. This document is to be signed by both the faculty supervisor and student and sent to the course coordinator by September 16<sup>th</sup>, 2019.

An example follows:

**Chemistry 402, "Semester"**  
**Student Name and UCID:**

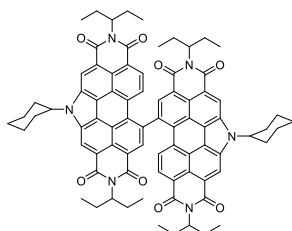
**Title:** Side-chain engineering of perylene diimide non-fullerene acceptors for improved solar cell performance

**Overview:** Organic solar cells are a viable clean energy technology. To facilitate commercialization high performance must be coupled with green device fabrication methods and low-cost, stable active layer materials. This project will build on recent advances in developing perylene diimide non-fullerene acceptors which are relatively easy to make, can be processed from greener solvents, and enable good performing polymer based organic solar cells. The overall goal is to improve the solar cell performance by creating a better active layer morphology.

**Objectives:** Synthesis of a new N-annulated perylene diimide (PDI) with cyclic side chains and test as a non-fullerene acceptor in organic solar cells. Materials with linear alkyl or benzyl side chains have lead to polymer solar cells with power conversion efficiencies from 5-7%. Limiting is the miscibility of PDI with the polymer donor and the ability for the PDI to form small highly crystalline domains. The hypothesis is that cyclic side chains will result in a different self-assembly of the PDI potentially giving high solar cell performance.

**Research:**

- (1) Synthesize the PDI compound in >200 mg. Fully characterize using <sup>1</sup>H, <sup>13</sup>C NMR spec (fully assigned), high resolution MS, and elemental analysis
- (2) Determine materials properties using UV/vis, PL, DSC, and TGA.
- (3) Grow a single crystal of the compound and determine crystal structure
- (4) Investigate self-assembly by making films using the processing additives DIO and DPE
- (5) Work with a device HQP to obtain solar cell performance
- (6) Compare to the n-hexyl derivative



**Literature:**

Small Methods, 2018, 2, 1800081, Solar RRL 2018, 2, 1800009, Advanced Functional Materials, 2011, 21, 1616-1623, Chemistry of Materials, 2005, 17, 3366-3374.

**Course Evaluation:**

- Create a detailed PowerPoint presentation that outlines the, project, literature, research goals, and work plan (25%)
- Research work (25%) – this is determined by faculty supervisor and graduate student mentor
- Interpretation of results (25%) – as determined by formal research updates using PowerPoint
- Final presentation to the research group (25%)

**Approval**

Faculty Supervisor Name and Signature: \_\_\_\_\_

Student Name and Signature: \_\_\_\_\_

All grades due to the course coordinator on or before December 19<sup>th</sup>, 2019.

Departmental approval: Electronically Approved

Date: September 3, 2019