



**UW DIRECT Capstone Project Proposal**

The project should allow fellows to accomplish three goals: 1) cement the acquisition of new Data Science skills, 2) develop proficiency in the conduct of team-based interdisciplinary research, and 3) enhance existing clean energy research in our institutions through the application of Data Science methods.

**PROJECT NAME:** Processing and Properties: Linking Thin Film Morphology to its Creation

**PROJECT DESCRIPTION:** The goal of this project is to begin to establish a relationship between the processing conditions used to make a thin film, the chemical characteristics of the polymer, and the morphology of the film. These connections are crucial for the progression of technologies using organic semiconductors, such as OPVs, OFETs, and OLEDs.

**DESCRIPTION OF DATA TO BE USED:** This project will make use of both published experimental data and generation of its own data and structural characterizations

**PROJECT START DATE:** 3/27/17

**PROJECT END DATE:** 12/27/17

**PROBLEM TO SOLVE/OBJECTIVE:**

Organic, thin-film technologies have made rapid progress in device efficiencies by focusing on chemical structures. However, the precise prediction of micro and macro-structure of the thin films is crucial for full implementation of these technologies. Film processing conditions can include concentration, solubility, and annealing, while chemical properties concern the polymer structure itself, e.g. molecular weight and back-bone rigidity.

The objective of this project is to quantify the effect that each parameter has on the thin-film structure. The relationships will be determined through statistical analysis, carried out by developing a Python framework, with the goal of producing a translatable framework for different polymers. Morphology will be characterized through XRD and SPM techniques.

**TIMELINES AND DELIVERABLES:** A rough outline of the expected work plan and deliverables is:

- Generate and obtain experimental data [To be performed by Luscombe lab // non-NRT trainee]
- Initial data processing through data visualization techniques
- Use Scikit-Image and Scikit learn to perform visual and statistical analysis and machine learning on dataset
- Finalize initial release of codebase, test data, and manuals
- Wrap-up and Presentation

The main deliverables will be a new software product (released for public use) for predicting morphology and a research paper of key findings, which the team hopes to publish in a peer-reviewed journal. By the end of the project period the team will deliver:

- Publication of software product and basic support documents on free open repository on GitHub
- A final written report that addresses the following:
  1. Effects of Processing conditions on thin film morphology
  2. Effects of polymer structure on thin film morphology
  3. Performance of regression methods on morphology characterization
  4. Discussion on the characterization of thin film morphology and its relationship to performance

Plots/visualizations of results/conclusions

**PROJECT LEADER:**

Wes Tatum

**PROJECT MENTOR(S):**

Prof. Christine Luscombe

**TEAM MEMBERS:** << we will fill >>