Christopher R. Collins

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Education

- **Carnegie Mellon University** — **Pittsburgh, PA**
  Ph.D. in Chemistry — *2014 – 2019 Expected*
- **University of North Georgia** — **Dahlonega, GA**
  B.S. in Chemistry with Chemical Physics Concentration — *2010 – 2014*

Research

- **Carnegie Mellon University** — **Pittsburgh, PA**
  Graduate Student; Advisor: David Yaron — *2014 – Present*
  - Optimizing INDO parameters using machine learning (Stochastic Gradient Descent, Parallel and Distributed Computing)
  - Examining coupling affects in polymeric systems of thiophene and phenyl (SPIE Paper)
  - Predicting optoelectronic properties of various polymeric systems using Deep Learning (10-701 term project)
  - Predicting molecular properties of various small molecules (Paper In Progress)
  - Advised undergraduate students in machine learning/python project
- **University of North Georgia** — **Dahlonega, GA**
  Undergraduate Researcher; Advisor: Aimée Tomlinson — *2011 – 2014*
  - Researched Benzobisazole Cruciforms structures using DFT for use as efficient organic solar cells
  - Designed and wrote set of tools to automate research process (Chemtools/Chemtools-webapp)
  - Instructed other group members about Unix and Gaussian usage methods
  - Led group members in structure studies (multicore systems, donor-acceptor systems, increased rings systems)
  - Used machine learning techniques to model data collected (Paper In Progress)
- **Carnegie Mellon University** — **Pittsburgh, PA**
  Undergraduate Researcher; Advisor: David Yaron — *Summer 2013*
  - Research into the decomposition of Thiaphospholes using DFT
  - Primary interest in the interactions of different substituents (thiophene, phenyl, furan)
  - Wrote MATLAB code to automate running Gaussian and AMPAC calculations and parsing results
  - Calculated molecular overlaps and generated molecular orbital diagrams
  - Created routines to draw structures with molecular orbital overlaps indicated on each atom

Work Experience

- **Tripwire, Inc.** — **Alpharetta, GA**
  Engineering Intern — *2012 – 2014*
  - Rewrote entire test suite for Benchmark product using Selenium and PyTest
  - Aided in migration of critical IP360 product and wrote automated test suite for API
  - Maintained and expanded installation automation for CCM product
  - Wrote automated script to test for CSRF and XSS vulnerabilities in IP360 product

Teaching

- Teaching Assistant
  - 09-221 Laboratory I: Introduction to Chemical Analysis
  - 09-214 Physical Chemistry
  - 09-101 Introduction to Experiemental Chemistry
  - 09-103 Atoms, Molecules, and Chemical Change
- Weekly Lecture Series in Theory Suite (Co-Started)
  - Intro to Python
  - Intro to Bash Scripting (2 lectures)
  - Intro to Object Oriented Programming
  - Intro to NumPy (2 lectures)

Publications

- **Collins, C. R.** ; Yaron, D. J. Constant Size Molecular Descriptors For Use With Machine Learning. *In Progress*.
- **Collins, C. R.** ; Tomlinson, A. L. Application of Machine Learning to Predict the Optoelectronic Properties of Benzobisazoles. *In Progress*.
- **Collins, C. R.** ; Yaron, D. J. Developing coarse-grained site models for excited electronic states of conjugated polymers. *SPIE* **2015**.
- Qiu, Y.; Worch, J. C.; Chirdon, D. N.; Kaur, A.; Maurer, A. B.; Amsterdam, S.; **Collins, C. R.** ; Pintauer, T.; Yaron, D.; Bernhard, S.; Noonan, K. J. T. Tuning Thiophene with Phosphorus: Synthesis and Electronic Properties of Benzobisthiaphospholes. *Chemistry A European Journal* **2014**.
- Tlach, B. C.; Tomlinson, A. L.; Morgan, K. D.; **Collins, C. R.** ; Jeffries-EL, M. Evaluation of the Impact of Extended Conjugation on the Optoelectronic Properties Benzo[1,2-d:4,5-d']bisoxazole Polymers. *Aust. J. Chem.* **2013**.

Presentations and Posters

- **Predicting Chemical Properties Using Machine Learning Methods** — **Farmington, PA**
  Department Retreat Poster Session — *2015*
- **The Influence of Chemical Representations on the Efficiency of Molecular Screening** — **Pittsburgh, PA**
  Graduate Seminar — *2015*
- **A Mission to Multivariate Adaptive Regression Splines (MARS) and Its Other-worldly Neighbors** — **Pittsburgh, PA**
  10-705 Statistical Machine Learning Term Project — *2015*
- **Predicting Chemical Properties Using Machine Learning Methods** — **Pittsburgh, PA**
  10-701 Intro to Machine Learning Term Project — *2014*
- **Application of Machine Learning to Predict the Optoelectronic Properties of Benzobisazoles** — **Dahlonega, GA**
  Senior Seminar — *2014*
- **Machine Learning in Chemical Compound Space** — **Dahlonega, GA**
  Junior Seminar — *2013*
- **Donor-Acceptor Behavior of Benzobisazole Cruciformic Polymers** — **Atlanta, GA**
  American Chemical Society Southeastern Regional Meeting — *2013*

- **The Impact of Conjugation Length on Benzobisazole Cruciforms** **Raleigh, NC**
  American Chemical Society Southeastern Regional Meeting *2012*
  - Runner-up Undergraduate Poster in Organic Chemistry

Technical Skills

Languages: Python, Javascript, C, C++ , MATLAB, Octave, Bash, Maple, CUDA C, TI-BASIC, SQL, Go, HTML, CSS, LaTeX, Mathematica, Java, Haskell

Software: *nix (Centos, BSD, various linux variants), Gaussian, LabVIEW, Git, SVN, SSH, rsync, coreutils, Make, Logisim

Libraries: Django, NumPy, SciPy, Matplotlib, Scikit-Learn, PyBrain, Selenium, Paramiko, PyTest, Twitter Bootstrap, jQuery, jQueryUI, SDL, OpenMP