Christopher R. Collins

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http://crcollins.com

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*
  - Optimized INDO parameters using machine learning with parallel and distributed computing
  - Examined coupling effects in polymeric systems of thiophene and phenyl
  - Predicted optoelectronic properties of various polymeric systems using Deep Learning
  - Developed new molecular descriptors for machine learning in chemistry
  - Advised undergraduate students in machine learning and Python
- **University of North Georgia** — **Dahlonega, GA**
  Undergraduate Researcher; Advisor: Aimée Tomlinson — *2011 – 2014*
  - Researched Benzobisazole Cruciform 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 usage methods
  - Led group members in structure studies (multicore systems, donor-acceptor systems, increased rings systems)
  - Developed machine learning model for predicting Benzobisazole properties
- **Carnegie Mellon University** — **Pittsburgh, PA**
  Undergraduate Researcher; Advisor: David Yaron — *Summer 2013*
  - Researched decomposition of Thiaphospholes using DFT
  - Wrote MATLAB code to automate running Gaussian/AMPAC calculations and parsing results
  - Wrote code to calculate molecular overlaps and generate 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 (Python)
  - 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 Experimental Chemistry (2 times)
  - 09-103 Atoms, Molecules, and Chemical Change
- Weekly Lecture Series in Theory Suite (Organizer)
  - Intro to Python
  - Intro to Bash Scripting (2 lectures)
  - Intro to Object Oriented Programming
  - Intro to NumPy (2 lectures)

Side Projects

- **Chemtools/Chemtools-Webapp** (`http://gauss.crcollins.com`)
  - Implemented a set of tools for use in Benzobisazole research
    - Gaussian log output parser to collect molecular properties
    - Machine learning model to predict polymer properties from oligomers
    - Benzobisazole structure generator and machine learning predictor for optoelectronic properties
    - Supercomputer job submitter and curator
  - Full automated testing suite (over 95% code coverage)
  - Python/Django Application with a Bootstrap front end
  - Vagrant VM build system
- **pyOS**
  - Implementation of a *nix like operating system using Python
  - Created shell similar to Bash Shell
  - Reimplemented standard unix programs (cp, mv, rm, ls, and etc)
  - Included permissions, pipes, multiple users, and a virtual file system
- **Other**
  - 8 bit CPU (Logisim)
  - Mandelbrot/Buddhabrot Generator (Python, Javascript, C/C++ , CUDA C, TI-BASIC)
  - Various Quadtree Visualizations (Python, C/C++ , Javascript)
  - Cellular Automata Based Electronic Simulation (Javascript)
  - Object Relation Management Library (Python/SQL)
  - University Course Scraper (Python)
  - Cryptography Library (Python, Logisim)
  - Automated Peer Review System Web Application (Python/Django)
  - Virtual Cluster and Server Architecture Vagrant Builds

Publications

- **Collins, C. R.** ; Gordon, G. J.; Yaron, D. J. Constant Size Molecular Descriptors For Use With Machine Learning. *Submitted to J. Chem. Theory Comput.*
- **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. *Chem. Eur. J.* **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**
  CMU Chemistry Department Retreat Poster Session — *2015*
- **The Influence of Chemical Representations on the Efficiency of Molecular Screening** — **Pittsburgh, PA**
  CMU Graduate Seminar — *2015*
- **A Mission to Multivariate Adaptive Regression Splines (MARS) and Its Otherworldly Neighbors** — **Pittsburgh, PA**
  CMU 10-702 Statistical Machine Learning Term Project — *2015*
- **Predicting Chemical Properties Using Machine Learning Methods** — **Pittsburgh, PA**
  CMU 10-701 Intro to Machine Learning Term Project — *2014*
- **Application of Machine Learning to Predict the Optoelectronic Properties of Benzobisazoles** — **Dahlonega, GA**
  UNG Senior Seminar — *2014*
- **Machine Learning in Chemical Compound Space** — **Dahlonega, GA**
  UNG 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, Mathematica, TI-BASIC, SQL, Go, HTML, CSS, LaTeX, Java, Haskell

Software: *nix (Linux, Centos, FreeBSD, AIX, Solaris), Gaussian/AMPAC, LabVIEW, Git, SVN, SSH, rsync, coreutils, Make, Logisim, ab, Vagrant, PostgreSQL, Varnish, nginx, Apache, Torque

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