CHRISTOPHER R. COLLINS

chris@crcollins.com
http://github.com/crcollins
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*

  – Developed parallel and distributed computing code for optimizing INDO parameters
  – 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 quantum computational methods
  – 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 web application

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, 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

Courses

- Linear Algebra (UNG)

- Intro to MATLAB (UNG)

- Intro to Cryptography (UNG)

- Differential Equations (UNG)

- Computational Methods in Physics (UNG)

- Into to Parallel Programming (Udacity)

- Convex Optimization (Stanford Online)

- Introduction to Machine Learning (CMU)

- Statistical Machine Learning (CMU)
- Graduate Artificial Intelligence (CMU)
- Quantum Chemistry (CMU)
- Special Topics in Computational Quantum Chemistry (CMU)
- Computational Chemistry (CMU)

Publications

- **Collins, C. R.**; Li, H.; Gordon, G. J.; Yaron, D. J. Continuous Bag of Bonds: A Size-Consistent Way of Representing Molecules. *Submitted*.

- **Collins, C. R.**; Gordon, G. J.; 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. *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

- **Constant Size Molecular Descriptors For Use With Machine Learning** Pittsburgh, PA
  Midwest Theoretical Chemistry Conference 2016

- **Constant Size Molecular Descriptors For Use With Machine Learning** Zürich, Switzerland
  CECAM Chemical Space Workshop 2016

- **Using Data to Accelerate Quantum Chemical Calculations by Getting Better at Guessing** Pittsburgh, PA
  CMU 15-780 Graduate Artificial Intelligence Term Project 2016

- **Using Machine Learning and Molecular Similarity to Predict Chemical Properties** Pittsburgh, PA
  CMU Progress Report 2016

- **Using Machine Learning and Molecular Similarity to Predict Chemical Properties** Pittsburgh, PA
  CMU Chemistry Department Poster Session 2016

- **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/HTML5, CSS, LaTeX, Java, Haskell, Ruby

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, OpenMPI