

Daniel C. Elton, Ph.D.

Skills

- Machine learning, natural language processing, molecular simulation, scientific writing and presentation
- Programming languages: Python, Matlab, Fortran
- Python libraries: numpy, matplotlib, scikit-learn, pandas, keras, gensim
- git, GNU/Linux, L^AT_EX, MacOS, MS Windows, MS Office
- limited experience: tensorflow, Bash, C++, Mathematica, openMP/openMPI, HTML

Experience

2018- **Assistant Research Scientist**, *University of Maryland, College Park*

Supervised by Prof. Peter W. Chung and Prof. Mark D. Fuge.

- Demonstrated for the first time that machine learning models can predict the properties of energetic molecules with high accuracy and low computational cost. (neural networks, ridge and LASSO regression, kernel ridge regression, random forest models, dimensionality reduction)
- Demonstrated how sensitivity analysis of machine learning models and feature ranking techniques can be used to help discover relationships between molecular structures and properties.
- Wrote a review article on deep learning architectures for molecular generation and demonstrated how a generative adversarial network can be used to generate sets of potentially useful molecules.
- Explained the utility of machine learning methods to program managers and chemists in DoD research labs.
- Supervised a masters student and four undergraduate students on a natural language processing project to extract chemical names, properties, and functionalities from large corpora of text extracted from pdfs and patent applications. Wrote code to calculate word2vec and GloVe embeddings and studied the clustering of chemical names in the word embedding space.

2017-2018 **Postdoctoral Associate**, *University of Maryland, College Park*, Same as above.

2018- **Talent**, *Mindfire Global*, Davos, Switzerland

- I was chosen as one of 36 “talents” out of hundreds of applicants to participate in the Mindfire program. Mindfire (www.mindfire.global) is a new initiative which brings together top talents in artificial intelligence, neuroscience, and other fields to help develop novel biologically inspired approaches to AI.

2012-2016 **Graduate Research Assistant**, *Stony Brook University*

Ph.D. adviser: Prof. Marivi Fernández-Serra

- Wrote a Fortran code (*PIMD-F90*) for quantum molecular dynamics simulation and a Python package (*spectrumfitter*) for fitting dielectric spectra. Parallelized code with MPI and ran large scale molecular dynamics simulations on HPC clusters.
- Gained extensive experience with Linux and cluster/supercomputer management.
- Planned and executed a detailed study of the dielectric properties of water which led to the discovery of optical phonon-like modes in liquid water. Published my work in Nature Communications.

2010-2012 **Graduate Teaching Assistant**, *Stony Brook University*

2010 **Summer Internship**, *Los Alamos National Laboratory*

- Worked with Dr. Garrett Kenyon on biologically-inspired neural networks for computer vision.

Education

Dec. 2016 **Ph.D. Physics**, *Stony Brook University*, Stony Brook, NY

Aug. 2009 **B.S., Physics**, *Rensselaer Polytechnic Institute*, Troy, NY
Mathematics minor, Magna Cum Laude, GPA 3.87

Publications

- 2018 **D. C. Elton**, Z. Boukouvalas, M. D. Fuge, and P. W. Chung. “Deep learning for molecular generation - a critical review of the state of the art”, in prep
- 2018 Z. Boukouvalas, **D. C. Elton**, M. D. Fuge, and P. W. Chung. “Independent Vector Analysis for Data Fusion Prior to Molecular Property Prediction with Machine Learning” Submitted to the 2018 Neural Information Processing Systems (NIPS) workshop on Machine Learning for Molecules and Materials.

- 2018 **D. C. Elton**, Z. Boukouvalas, M. S. Butrico, M. D. Fuge, and P. W. Chung, "Applying machine learning techniques to predict the properties of energetic materials", *Scientific Reports* **8**, 9059
- 2018 Z. Boukouvalas, **D. C. Elton**, M. D. Fuge, and P. W. Chung. "Independent Vector Analysis for Data Fusion Prior to Molecular Property Prediction with Machine Learning" Submitted to 2018 Neural Information Processing Systems (NIPS) workshop on Machine Learning for Molecules and Materials. (arXiv:1822.00628)
- B. C. Barnes, **D. C. Elton**, Z. Boukouvalas, D. E. Taylor, W. D. Mattson, M. D. Fuge, and P. W. Chung, "Machine Learning of Energetic Material Properties", 16th International Detonation Symposium, Cambridge MD (arXiv:1807.06156)
- 2018 F. G. VanGessel, G. Kumar, **D. C. Elton**, and P. W. Chung, "A Phonon Boltzmann Study of Microscale Thermal Transport in α -RDX Cook-Off", 16th International Detonation Symposium, Cambridge MD (arXiv:1808.08295)
- 2018 **D. C. Elton**, M. Fritz, and M.-V. Fernández-Serra, "Using a monomer potential energy surface to perform approximate path integral molecular dynamics simulation of ab-initio water at near-zero added cost" (arXiv:1803.05740, under review)
- 2017 **D. C. Elton** "The origin of the Debye relaxation in liquid water and fitting the high frequency excess response" *Phys. Chem. Chem. Phys.*, **19**, 18739
- 2016 **D. C. Elton** and M.-V. Fernández-Serra, "The hydrogen-bond network of water supports propagating optical phonon-like modes", *Nature Communications*, **7**, 10193
- 2014 **D. C. Elton** and M.-V. Fernández-Serra, "Polar nanoregions in water - a study of the dielectric properties of TIP4P/2005, TIP4P/2005f and TTM3F", *The Journal of Chemical Physics*, **140**, 124504
- 2010 M. A. Forman, C. W. Smith, B. J. Vasquez, B. T. MacBride, J. E. Stawarz, J. J. Podesta, **D. C. Elton**, U. Y. Malecot, and Y. Gagne. "Using Third-Order Moments of Fluctuations in V and B to Determine Turbulent Heating Rates in the Solar Wind.", *AIP Conference Proceedings*, *12th International Solar Wind Conference*, **1216**, 176
- 2009 J. J. Podesta, M. A. Forman, C. W. Smith, **D. C. Elton**, and Y. Malecot, "Accurate Estimation of Third-Order Moments from Turbulence Measurements", *Nonlin. Proc. Geophys*, **16**, 99

Professional development & service

- 2016-2017 Founder & Organizer, Tech Valley Machine Learning, Data Science, & AI Meetup
I hosted 18 meetups on topics in data science and machine learning, three of which were talks I gave myself. I have also given a talk entitled "Machine Learning Pitfalls" at meetups in Silver Spring, MD and Bellevue, WA.
- 2015- Peer Review Reviewer
I have reviewed for *Neural Computing and Applications*, *Journal of Physics Communications*, *Scientific Reports*, *Journal of Chemical Physics*, and *The Journal of Physical Chemistry Letters*.
- 2015-2016 Writer & Public Relations Director, *Stony Brook Frontiers* magazine
- 2013-2015 Senator & Social Concerns Committee member, Stony Brook Graduate Student Organization
- 2014-2015 Volunteer, Stony Brook Astronomy Open Nights
- 2014,2015 Judge, Nassau County Science Competition
- 2012 Improvisation for Scientists Course, Alda Center for Communicating Science

Honors

- | | |
|-----------------------------------|--|
| 2014 Peter B. Kahn travel prize | 2006 Willits Foundation Scholarship |
| 2009 Rensselaer Founder's Award | 2006 RIT Computing Award/Scholarship |
| 2008 Sigma Pi Sigma | 2006 National Merit Scholarship Finalist |
| 2006 Rensselaer Medal/Scholarship | 2004 Eagle Scout Award |

References

- o Prof. Peter W. Chung, pchung15@umd.edu, 613-520-2600 x-5703
- o Prof. Mark D. Fuge, fuge@umd.edu, 301-405-2558
- o Prof. Marivi Fernández-Serra, maria.fernandez-serra@stonybrook.edu, 631-632-8244
- o Prof. Philip B. Allen, philip.allen@stonybrook.edu 631-632-8179