

Daniel C. Elton

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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

Recent Experience

2017- **Postdoctoral Associate**, *University of Maryland, College Park*

Working with Prof. Mark Fuge and Prof. Peter W. Chung studying applications of machine learning to molecular design and discovery. My research has covered several different thrusts of exploration:

- Targeted lead generation - research on deep learning architectures for molecular generation and optimization (variational autoencoders, generative adversarial networks)
- Molecular property prediction - using custom molecular featurization techniques and machine learning models to predict the properties of energetic molecules. (ridge and LASSO regression, kernel ridge regression, neural networks, random forest models)
- Structure-property relationships - exploring data mining methods and methods of interpreting machine learning models to discovery molecular structure-property relationships. (model sensitivity analysis, feature importance ranking)
- Natural language processing - currently supervising a masters student and two undergraduate students who are using NLP techniques to identify keywords in scientific documents and extract chemical names. Exploring word embedding techniques and sentence parsing to identify chemicals and their properties. (TF-IDF, word2vec, word clouds, named entity recognition)

Feb-Apr 2017 **Tutor**, *Schenectady County Community College*

- Tutor in the Learning Center for physics, chemistry, and math.

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

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

- Wrote thousands of lines of code in Python and Fortran for quantum molecular dynamics simulation, analyzing molecular dynamics trajectories, and fitting spectra. Parallelized code with MPI.
- Planned and executed a detailed study of the dielectric spectra of water which led to the discovery of optical phonon-like modes in liquid water.
- Ran molecular dynamics simulations with thousands of molecules on HPC clusters.
- Wrote the *spectrumfitter* Python package for fitting dielectric spectra.

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.

2009-2010 **Graduate Teaching Assistant**, *Rensselaer Polytechnic Institute*

2008-2009 **Undergraduate Research Assistant**, *Rensselaer Polytechnic Institute*

2008 **Summer Research Experience for Undergraduates**, *Stony Brook University*

Computer skills

- Fortran (6 years), Matlab (5 years), Python (4 years), Mathematica (2 years)
 - beginner level: C, openMP/openMPI, Bash, HTML
 - L^AT_EX, Git, *scikit-learn*, *keras*, *tensorflow*
 - GNU/Linux, MacOS, MS Windows, MS Office, EndNote
- code examples at www.github.com/delton137

Publications

- 2018 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, (abstract accepted, in prep)

- 2018 F. G. VanGessel, **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, (abstract accepted, in prep)
- 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" (arXiv:1801.04900, under review)
- 2018 **D. C. Elton** and M. Fritz "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, in prep)
- 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
- 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

Honors

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| 2018 Talent, MindFire Mission-1 | 2006 Willits Foundation Scholarship |
| 2014 Peter B. Kahn travel prize | 2006 RIT Computing Award/Scholarship |
| 2009 Rensselaer Founder's Award | 2006 National Merit Scholarship Finalist |
| 2008 Sigma Pi Sigma | 2004 Eagle Scout Award |
| 2006 Rensselaer Medal/Scholarship | |

Professional development & service

- 2016-2017 Founder & Organizer, Tech Valley Machine Learning, Data Science, & AI Meetup
- 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
- I am a registered and active peer reviewer for *Neural Computing and Applications*
- Over the years I have reviewed or assisted in reviews for:
- *Journal of Physics Communications*
 - *Scientific Reports*
 - *Journal of Chemical Physics*
 - *The Journal of Physical Chemistry Letters*

Talks

- 6-03-18 Gordon Research Seminar - Advances in Modeling, Experimental Developments and Synthesis of Energetic Materials, *Newry, Maine*
Invited talk: "Machine Learning for Design and Discovery of New Energetic Materials"
- 4-20-18 Army Research Laboratory, *Aberdeen, Maryland*
Invited talk: "Machine Learning of Energetic Molecule Performance"
- 2-21-18 Artificial Intelligence Information Meetup, *Silver Spring, Maryland*
"Pitfalls of Machine Learning"
- 2-10-18 Bellevue Machine Learning & Artificial Intelligence Meetup, *Bellevue, Washington*
"Pitfalls and Biases in Machine Learning"

- 12-28-17 Tech Valley Machine Learning Meetup, *Troy, New York*
"Machine learning pitfalls"
- 11-20-17 Tech Valley Machine Learning Meetup, *Troy, New York*
"Interpretable machine learning for molecular design and discovery"
- 12-12-16 Tech Valley Machine Learning Meetup, *Troy, New York*
"Scikit-learn & Keras applied to digit recognition"
- 3-16-16 American Physical Society March Meeting, *Baltimore, Maryland*
"Accurate path integral molecular dynamics simulation of *ab-initio* water at near-zero added cost"
- 2-3-16 Institute for Advanced Computational Science, *Stony Brook University*
Invited talk: "Propagating Optical-Phonon Like Modes in Liquid Water"
- 11-27-15 Young Researcher Symposium, *Brookhaven National Lab*
"Propagating optical phonon-like modes in liquid water"
- 3-2-15 American Physical Society March Meeting, *San Antonio, Texas*
"Exploring the nonlocal dielectric susceptibility of liquid water in the terahertz regime - propagating modes, Debye relaxation, and overscreening"
- 7-26-14 Gordon Research Seminar - Water & Aqueous Solutions, *Holderness School, NH*
Invited talk: "Water - a Relaxor Ferroelectric?"
- 4-17-14 Graduate Student Friday Afternoon Seminar, *Stony Brook University*
"Water - a Relaxor Ferroelectric?"
- 3-5-14 American Physical Society March Meeting, *Denver, Colorado*
"Polar nanoregions in water - a study of the dielectric properties of TIP4P/2005, TIP4P2005f and TTM3F"

Poster presentations

- 2-5-18 New Deep Learning Techniques, *Institute for Pure and Applied Mathematics*
"Interpretable machine learning for molecular property prediction and discovery"
- 6-29-17 Machine Learning for Materials Research Workshop, *University of Maryland*
"Fitting and Understanding the Dielectric Spectra of Liquid Water"
- 4-13-16 Institute for Advanced Computational Sciences Research Day, *Stony Brook University*
"The H-bond network of liquid water supports propagating phonons"
- 3-17-16 American Physical Society March Meeting, *Baltimore, Maryland*
"The hydrogen bond network of water supports propagating optical phonon-like modes"
- 10-23-15 Chemistry Research Day, *Stony Brook University*
"The H-bond network of liquid water supports propagating phonons"
- 9-18-15 Institute for Advanced Computational Science Grand Opening, *Stony Brook University*
"The H-bond network of liquid water supports propagating phonons"
- 7-29-14 Gordon Research Conference - Water & Aqueous Solutions, *Holderness School, NH*
"Water - a Relaxor Ferroelectric?"
- 3-21-14 5th New York Theoretical and Computational Chemistry Conference, *Stony Brook University*
"Polar nanoregions in water - a study of the dielectric properties of TIP4P/2005, TIP4P/2005f and TTM3F"
- 1-14-13 4th New York Theoretical & Computational Chemistry Conference, *City University of New York*
"The Dielectric Properties and Dipolar Correlations of Liquid Water Investigated using TIP4P/2005 Rigid and Flexible Models"
- 11-6-12 8th Gotham-Metro Condensed Matter Meeting, *New York Academy of Sciences*
"The Dielectric Properties and Dipolar Correlations of Liquid Water Investigated using TIP4P/2005 Rigid and Flexible Models"