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 - researched and tested recently proposed deep learning architectures for molecular generation and optimization - variational autoencoders and generative adversarial networks.
- Molecular property prediction - used custom molecular featurization techniques and machine learning models to predict the properties of energetic molecules.
- Discovery of structure-property relationships - compared the usefulness of statistical dependency tests, feature ranking techniques, and sensitivity analysis of machine learning models to the discovery of molecular structure-property relationships.
- Natural language processing - supervised a masters student and undergraduate student who used basic NLP techniques to identify keywords in scientific documents and extract chemical names.

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
- LaTeX, 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

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

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

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 Meetuptup, *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*
Poster: "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*
Poster: "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"

References

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Prof. Philip B. Allen
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