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Daniel C. Elton

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 three main thrusts:

- Molecular property prediction - using custom molecular featurization techniques and machine learning models to accurately predict the properties of energetic molecules.
- Data mining structure-property relationships - rigorous application of statistical dependency tests, feature ranking techniques, and sensitivity analysis of machine learning models to discover molecular structure-property relationships.
- Targeted lead generation - developing systems for molecular generation and optimization using deep learning architectures - variational autoencoders and generative adversarial networks.

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.
- 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.
- Parallelized my custom path integral molecular dynamics code with MPI.
- 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
- 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**, 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" (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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|-----------------------------------|--|
| 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 |

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

- 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*
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

Prof. Peter W. Chung

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Prof. Mark D. Fuge

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Prof. Marivi Fernández-Serra

Stony Brook University

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Prof. Philip B. Allen

Stony Brook University

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