

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

Experience

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

I am supervised by Prof. Peter W. Chung and Prof. Mark D. Fuge. My research at UMD has covered several different thrusts of exploration:

- Molecular property prediction with machine learning (neural networks, ridge and LASSO regression, kernel ridge regression, random forest models, dimensionality reduction)
- Structure-property relationships - have published on methods of interpreting machine learning models to discover molecular structure-property relationships. (model sensitivity analysis, feature importance ranking)
- Molecular generation with deep learning architectures (variational autoencoders, generative adversarial networks)
- Natural language processing - for past 6 months I have been supervising a masters student and three undergraduate students who are exploring NLP approaches to extracting chemical names, properties, and functionalities from large collections of pdfs. I personally have written code to visualize and explore the word embeddings of chemical names.

2018- **Talent**, *Mindfire Global*

- I was chosen as one of 36 "talents" out of hundreds of applicants to participate in the inaugural Mindfire mission in Davos, Switzerland in May 2018. Mindfire (www.mindfire.global) is a new program which brings together top talents in artificial intelligence, neuroscience, and many other fields to brainstorm new ways of creating biologically inspired AI. The next mission will be in spring 2018.

2017-2018 **Postdoctoral Associate**, *University of Maryland, College Park*

Spring 2017 **STEM Tutor**, *Schenectady County Community College*

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

- Core languages: Python, Fortran, Matlab
 - limited working proficiency: C, Mathematica, openMP/openMPI, HTML
 - Python libraries: *numpy*, *matplotlib*, *scikit-learn*, *pandas*, *keras*
 - \LaTeX , Git, 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 (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**, 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 **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

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 have reviewed for:
- *Neural Computing and Applications*
 - *Journal of Physics Communications*
 - *Scientific Reports*
 - *Journal of Chemical Physics*
 - *The Journal of Physical Chemistry Letters*
- (see details, see my Publons profile)

Talks

- 9-21-18 Deep Learning RIT (Research Interaction Team), *UMD Mathematics Department, College Park, Maryland*
 "Introduction to machine learning topics : optimization techniques and convolutional neural networks"
- 8-2-18 Visit of SEAP interns from Indian Head Naval Surface Warfare Center, *College Park, Maryland*
 Invited talk: "Machine Learning and AI for Navy Energetics"
- 6-7-18 Talk to Gad Getz's group at the Broad Institute, *Cambridge, Massachusetts*
 "Machine Learning for Design and Discovery of New Energetic Materials"
- 6-3-18 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

- 9-17-18 Postdoctoral Research Symposium, *University of Maryland, College Park*
 "Machine learning for molecular property prediction and discovery"
- 8-7-18 Artificial Intelligence for Materials Science (AIMS) Workshop, *NIST, Gaithersburg, Maryland*
 "Machine learning for molecular property prediction and discovery"
- 6-3-18 Gordon Research Seminar - Advances in Modeling, Experimental Developments and Synthesis of Energetic Materials, *Newry, Maine*
 "Machine learning for molecular property prediction and discovery"
- 2-5-18 New Deep Learning Techniques Workshop, *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"

References

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