

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. Peter W. Chung and Prof. Mark Fuge applying machine learning to molecular design. Studying molecular property prediction, molecular fingerprinting/featurization, and lead generation with variational autoencoders and Bayesian optimization.
- 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
- Developed programming and code management skills by writing thousands of lines of code in Python and Fortran for quantum molecular dynamics simulation, analyzing molecular dynamics trajectories, and spectrum fitting.
 - Planned and executed a detailed study of the dielectric spectra of water which led to the discovery of phonon-like modes in liquid water.
 - Ran molecular dynamics simulations with thousands of molecules on HPC clusters.
 - Parallelized my custom path integral molecular dynamics (PIMD) code with MPI.
 - Developed a novel algorithm that speeds up PIMD simulation with density functional theory by a factor of 30 with acceptable losses in accuracy.
 - 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*
- 2009 **Undergraduate Research Assistant**, *Rensselaer Polytechnic Institute*
- 2008-2009 **Undergraduate Research Assistant**, *Rensselaer Polytechnic Institute*
- 2008 **Research Experience for Undergraduates**, *Stony Brook University*

Computer skills

- Fortran (5 years), Python (3 years), Matlab (4 years)
- MP/MPI, C, Bash, HTML, Mathematica
- L^AT_EX, Git, GROMACS, SIESTA, VASP, Jmol, VMD
- GNU/Linux, MacOS, MS Windows, MS Office

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

Publications

- 2017 **D. C. Elton** "The origin of the Debye relaxation in liquid water and fitting the high frequency excess response" arXiv:1704.01667 *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

Talks

- 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?"
3-5-14 American Physical Society March Meeting, *Denver, Colorado*
"Polar nanoregions in water - a study of the dielectric properties of TIP4P/2005, TIP4P/2005f and TTM3F"
4-17-14 Graduate Student Friday Afternoon Seminar, *Stony Brook University*
"Water - a Relaxor Ferroelectric?"

Poster presentations

- 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. Marivi Fernández-Serra

Stony Brook University

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Prof. Phil Allen

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Prof. Matthew Dawber

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Prof. Robert Harrison

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