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 studying applications of machine learning to molecular property prediction and molecular design.

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
- LaTeX, Git, GROMACS, SIESTA, VASP, Jmol, VMD
- GNU/Linux, MacOS, MS Windows, MS Office

Honors

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

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

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
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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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