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# ADRIAN W. LANGE

SCIENTIST + PROGRAMMER

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## SUMMARY

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- Broad physical science background
- Strong computer programming skills
- Productive record of achievement

## TECHNICAL SKILLS

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- **Proficient:** C++, C, Python, Unix/Linux shell, awk, OpenMP, MPI,  $\text{\LaTeX}$
- **Familiar:** Java, Fortran, SQL, Perl, Pthreads, CUDA, HTML, CSS, JavaScript, CVS, SVN, Octave

## EMPLOYMENT

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<b>Postdoctoral Appointee</b>	<b>Argonne National Laboratory Leadership Computing Facility</b>	<b>March 2012 – Present</b>
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- Researched simulations of chemically reactive force fields and proton transport dynamics
- Developed code/algorithms for novel massively parallel simulations on IBM Blue Gene/Q supercomputer, Mira
- Increased code speed more than 8x, scalability to  $\sim 0.4$  million cores

<b>Ph.D. Student Researcher</b>	<b>The Ohio State University</b>	<b>June 2007 – March 2012</b>
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- Researched quantum mechanical simulations of photoexcited DNA and solvent electrostatics
- Published 10 first author journal articles, 230+ total citations, h-index 6 (for listing, see my [Google Scholar Citations](#))
- Presented research orally over 20 times at professional events/conferences
- Led recitations and conducted exams as teaching assistant for physical chemistry courses

## EDUCATION

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<b>Columbus, OH</b>	<b>The Ohio State University</b>	<b>June 2007 – March 2012</b>
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- **Ph.D.** Computational/Physical Chemistry (GPA: 3.65) Advisor: Prof. John M. Herbert

<b>Columbus, OH</b>	<b>The Ohio State University</b>	<b>August 2003 – June 2007</b>
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- **B.S.** Chemistry with minor in Microbiology (GPA: 3.39)

### Coursework:

- **Graduate/Undergraduate:** Quantum mechanics, Statistical mechanics, Computational chemistry, Multivariable calculus, Linear algebra, Differential equations, Computer programming, Numerical methods, Parallel computing
- **Supplemental online:**
  - **Coursera:** Machine learning, Data science, Algorithms, Databases
  - **Udacity:** Web development, GPU programming, Programming languages

## ADDITIONAL TECHNICAL EXPERIENCE/PROJECTS

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- **Q-Chem v4.0** (2009–2013): Lead author of polarizable continuum model and QM/MM codes in commercial software package, [Q-Chem](#); software design committee member (C++, C, Fortran)
- **LAMMPS Ensembles** (2013): Multi-copy communication interface to open-source software, [LAMMPS](#); contributions to main LAMMPS source code (C++, C, MPI, OpenMP, Python)
- **FMR** (2013): Reactive quantum fragment simulator; interfaced with Q-Chem (Python, C++, MPI)
- **DESMO** (2011): Highly parallel solvent model code; genetic algorithm dynamic load balancing (C++, OpenMP, MPI)

## HONORS AND AWARDS

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- Presidential Fellowship from The Ohio State University Graduate School (2011–2012; \$33,150)
- Chemical Computing Group Research Excellence Award from American Chemical Society (2012; \$1,150)
- U.S. Department of Energy Merit Scholarship for top poster presentation (2010; \$400)
- American Society for Microbiology Undergraduate Research Fellowship (2006; \$4,000)
- Ohio State Arts & Sciences Undergraduate Honors Research Scholarship (2006; \$3,500)