# NATHAN WALTER

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#### **EDUCATION**

#### University of Illinois at Champaign-Urbana (UIUC)

08.2013 - presentPhD Candidate in Nuclear, Plasma, and Radiological Engineering (NPRE) Expected: 08.2018 Master of Science in Nuclear, Plasma, and Radiological Engineering (NPRE) 08.2018

Graduate Minor in Computational Science and Engineering

Advisor: Yang Zhang

• Master's Thesis Topic: Direct Energy Landscape Sampling of the Homogeneous Nucleation and Crystal Growth of a Model Liquid

## University of Illinois at Champaign-Urbana (UIUC)

08.2010 - 12.2014

Bachelor of Science in Nuclear, Plasma, and Radiological Engineering (NPRE)

Overall GPA: 3.84/4.00 Minor in Mathematics

#### AWARDS, HONORS, CLUBS, AND CERTIFICATES

American Physical Society, GSOFT Travel Award 03.2017 Graduate Specialization in Computational Science and Engineering 08.2016 Los Alamos National Lab Computational Summer Workshop 06.2014 - 08.2014U.S. Department of Energy, Naval Reactors (NR), Rickover Fellowship Program Honorable Mention 00.2014 Nuclear Regulatory Commission Undergraduate Scholarship 12.2011 - 06.2013University of Illinois at Champaign-Urbana Dean's List Recipient 06.2011 - 0.62013The Hacker Within, An organization for computational scientists. Member: 08.2015 – present Treasure: 08.2016 - present

#### SELECT PRESENTATIONS AND PUBLICATIONS

Talk, American Physical Society March Meeting, "Protein Folding and Unfolding Dynamics from Direct Energy Landscape Sampling Simulations" 03.2017

Talk, University of Illinois Urbana-Champaign Nuclear Engineering Undergraduate Seminar, "Homogeneous Nucleation and Crystal Growth in a Model Liquid from Direct Energy Landscape Sampling Simulations"

Tim P. MoneyPenny II, Nathan Walter, Zhikun Cai, Y. Miao, D. Gray, J. Hinman, S. Lee, Yang Zhang, Jeff Moore, "Impact of shape persistence on the porosity of molecular cages" J. Am. Chem. Soc (2017).

Nathan Walter, Paul Friedrichsen, Scott Runnels, "Extending a Strain Space Formulation for Plasticity to Rate-Hardening Materials and Finite Rotations", LA-UR-15-23329, Los Alamos Unlimited Release (2015).

#### TECHNICAL STRENGTHS

Software

C, C++, Matlab, Python, Fortran, Java, LATEX, Swift (novice), Computer Programming Languages AJAX, R, OpenMP, MPI, HTML, CSS, Julia (novice), Make

GROMACS, LAMMPS, VASP, SRIM/TRIM, FLAG,

VMD, IGOR Pro, Dave, gnuplot, Adobe Suite, SPSS

### SELECT RESEARCH PROJECTS

- Implemented a metadynamics method for directly sampling the energy landscape into the molecular dynamics package GROMACS, studied the activation barrier statistics of amorphous and ordered systems
- Developed an open-source package, LiquidLib, to analyze molecular dynamics trajectories to study the structure and dynamics of liquids and compare the results to neutron scattering experiments
- Performed ab initio molecular dynamic simulations to study the vibrational modes in D<sub>2</sub>O, the effects of hydrogen impurities on liquid lithium transport properties, and shape persistence in molecular cages
- Created a high dimensional molecular dynamics package to study the dimensionality of various quantities