Josh Vermaas

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Education

2016 **Ph.D. in Biophysics**, *University of Illinois at Urbana-Champaign*, Thesis title: Interfacial modulation of protein function explored through atomistic molecular dynamics simulation.

2010 **B.S. in Physics, Biochemistry, and Computational Math**, *Arizona State University*, summa cum laude.

Research Experience

2020–Present **Computational Scientist**, *Oak Ridge Laboratory*, Oak Ridge, TN.
INCITE liaison for NAMD-related projects, and ensuring application readiness for NAMD on upcoming supercomputing systems.

2016–2019 **Director's Postdoctoral Fellow**, *National Renewable Energy Laboratory*, Golden, CO.
Postdoctoral work under the mentorship of Michael Crowley and Gregg Beckham, with a number of projects, principally related to lignin utilization,[1–3,5,7] membrane permeability,[3,8,10] and enzyme structure and mechanism.[4,6]

2010-2016 **Graduate Student**, *University of Illinois at Urbana-Champaign*, Urbana, IL.
Graduate research performed with Emad Tajkhorshid as advisor. Research projects include methods development[11,15,20,25] and application[12,24,26] of accelerated and conventional[12,13,17,18] membrane models, adding capabilities to the molecular dynamics visualization program VMD,[16] and simulations related to interactions within the photosynthetic reaction center of *Rhodobacter sphaeroides*[23] or cytochrome bo_3.[14]

Fall 2015 **Sandia Graduate Fellow**, *Sandia National Laboratory*, Albuqueque, NM.
On-site research supervised by Susan Rempe on the connection between substrate loading conditions and conformational change in the antibiotic resistance transporter EmrE.[9]

Summer 2014 **Computational Science Graduate Fellow**, *Oak Ridge National Laboratory*, Oak Ridge, TN.
Analyzed a microsecond long multimillion atom lignocellulose system under the supervision of Loukas Petridis and Jeremy Smith, including novel visualization techniques.[19]

Summer 2012 **Computational Science Graduate Fellow**, *National Renewable Energy Laboratory*, Golden, CO.
Developed and applied force fields for oxidized carbohydrates to gague their impact on cellulose decrystallization and cellulase inhibition.[22] Supervised by Gregg Beckham, Michael Crowley, and Christina Payne.

2007-2010 **Undergraduate Researcher**, *Arizona State University*, Tempe, AZ.
Diverse projects across the physics department to gague my interests across research fields and techniques,[27] with supervision by Bruce Doak and Ralph Chamberlin. Projects in biology included a research thesis developing computational kinetic models based on experimentally determined metabolic fluxes.

Grantwriting Experience (Funded proposals underlined)

Money

2010 DOE Computational Sciences Graduate Fellowship PI: Josh Vermaas
2010 NSF Graduate Research Fellowship PI: Josh Vermaas
2011,2016 NIH P41 Center Renewal Proposal PI: Klaus Schulten
2011-2016 NIH R01 proposals PI: Emad Tajkhorshid
2012 NSF Project Funding PI: Emad Tajkhorshid
2014 Sandia Excellence in Science & Engineering Graduate Fellowship PI: Josh Vermaas
2015 NREL Director's Postdoctoral Fellowship PI: Josh Vermaas
2015 ORNL Wigner Postdoctoral Fellowship PI: Josh Vermaas
2015 Sandia Truman Postdoctoral Fellowship PI: Josh Vermaas
2018 NREL Laboratory Directed Research and Development PI: Josh Vermaas
2019 NREL Laboratory Directed Research and Development PI: Eric Karp

Computer Time

2011-2015 XSEDE/Teragrid Allocation Proposals PI: Emad Tajkhorshid
2014-2016 NERSC Compute Allocation PI: Josh Vermaas
2015 INCITE Allocation Proposal PI: Emad Tajkhorshid
2016-2019 XSEDE Allocation Proposals PI: Gregg Beckham
2016-2019 Internal NREL Allocation Proposal PI: Mike Crowley

Postgraduate Awards

2016-2019 Director's Postdoctoral Fellow, National Renewable Energy Laboratory
2018 Wiley Computing in Chemistry Outstanding Postdoc Award
2014-2016 Sandia National Laboratories Excellence in Science and Engineering Research Program Fellowship
2011-2014 DOE Computational Sciences Graduate Fellowship
2010-2011 NIH Biophysics Trainee

Service

2017-2019 Special awards and physics judge for the Denver Metro and Washington/Morgan Bicounty science fairs

2018-2019	Scorekeeper or moderator for the Colorado regional high school science bowl
2016-2019	Reviewer for several ACS, RSC, and MDPI journals

Programming Languages

C/C++	Primary medium for changes to VMD or Colvars	Python	Day to day glue language for simulation analysis
Tcl	Preferred for simulation setup	CUDA	GPU acceleration of analysis bottlenecks
Java	Academic and portable codes	OpenMP and MPI	Multicore and multinode coding frameworks

Biomolecular Simulation Toolset

Molecular visualization tools	VMD, pymol, Chimera
Molecular dynamics engines	NAMD, GROMACS, CHARMM, and Amber
Sampling techniques	Metadynamics, Umbrella sampling, alchemical transformations, Hamiltonian replica exchange
Analysis tools and libraries	VMD, MDAnalysis, NetworkX, scipy, rdkit
Experimental comparison tools	ShiftX, Camshift, Molprobity, (x)MDFF
Force field parameter optimization	CGenFF, FFTK

Languages

English	Native and scientific
Dutch	Native
German	6th grade level

Publications

(1) Orella, M. J.; Gani, T. Z. H.; Vermaas, J. V.; Stone, M. L.; Anderson, E. M.; Beckham, G. T.; Brushett, F. R.; Román-Leshkov, Y. Lignin-KMC: A Toolkit for Simulating Lignin Biosynthesis. *ACS Sustain. Chem. Eng.* **2019**, *7*, 18313–18322, DOI: 10.1021/acssuschemeng.9b03534.

(2) Vermaas, J. V.; Crowley, M. F.; Beckham, G. T. A Quantitative Molecular Atlas for Interactions Between Lignin and Cellulose. *ACS Sustain. Chem. Eng.* **2019**, acssuschemeng.9b04648, DOI: 10.1021/acssuschemeng.9b04648.

(3) Vermaas, J. V.; Dixon, R. A.; Chen, F.; Mansfield, S. D.; Boerjan, W.; Ralph, J.; Crowley, M. F.; Beckham, G. T. Passive membrane transport of lignin-related compounds. *Proc. Natl. Acad. Sci.* **2019**, *116*, 23117–23123, DOI: 10.1073/pnas.1904643116.

(4) Vermaas, J. V.; Kont, R.; Beckham, G. T.; Crowley, M. F.; Gudmundsson, M.; Sandgren, M.; Ståhlberg, J.; Väljamäe, P.; Knott, B. C. The dissociation mechanism of processive cellulases. *Proc. Natl. Acad. Sci.* **2019**, *116*, 23061–23067, DOI: 10.1073/pnas.1913398116.

(5) Vermaas, J. V.; Dellon, L. D.; Broadbelt, L. J.; Beckham, G. T.; Crowley, M. F. Automated Transformation of Lignin Topologies into Atomic Structures with LigninBuilder. *ACS Sustain. Chem. Eng.* **2019**, *7*, 3443–3453, DOI: 10.1021/acssuschemeng.8b05665.

(6) Zheng, F.; Vermaas, J. V.; Zheng, J.; Wang, Y.; Tu, T.; Wang, X.; Xie, X.; Yao, B.; Beckham, G. T.; Luo, H. Activity and Thermostability of GH5 Endoglucanase Chimeras from Mesophilic and Thermophilic Parents. *Appl. Environ. Microbiol.* **2019**, *85*, e02079–18, DOI: 10.1128/AEM.02079-18.

(7) Vermaas, J. V.; Petridis, L.; Ralph, J.; Crowley, M. F.; Beckham, G. T. Systematic parameterization of lignin for the CHARMM force field. *Green Chem.* **2019**, *21*, 109–122, DOI: 10.1039/C8GC03209B.

(8) Vermaas, J. V.; Bentley, G. J.; Beckham, G. T.; Crowley, M. F. Membrane Permeability of Terpenoids Explored with Molecular Simulation. *J. Phys. Chem. B* **2018**, *122*, 10349–10361, DOI: 10.1021/acs.jpcb.8b08688.

(9) Vermaas, J. V.; Rempe, S. B.; Tajkhorshid, E. Electrostatic lock in the transport cycle of the multidrug resistance transporter EmrE. *Proc. Natl. Acad. Sci.* **2018**, *115*, E7502–E7511, DOI: 10.1073/pnas.1722399115.

(10) Vermaas, J. V.; Beckham, G. T.; Crowley, M. F. Membrane Permeability of Fatty Acyl Compounds Studied via Molecular Simulation. *J. Phys. Chem. B* **2017**, *121*, 11311–11324, DOI: 10.1021/acs.jpcb.7b08233.

(11) Vermaas, J. V.; Pogorelov, T. V.; Tajkhorshid, E. Extension of the Highly Mobile Membrane Mimetic to Transmembrane Systems through Customized in Silico Solvents. *J. Phys. Chem. B* **2017**, *121*, 3764–3776, DOI: 10.1021/acs.jpcb.6b11378.

(12) Vermaas, J. V.; Tajkhorshid, E. Differential Membrane Binding Mechanics of Synaptotagmin Isoforms Observed in Atomic Detail. *Biochemistry* **2017**, *56*, 281–293, DOI: 10.1021/acs.biochem.6b00468.

(13) Mayne, C. G.; Arcario, M. J.; Mahinthichaichan, P.; Baylon, J. L.; Vermaas, J. V.; Navidpour, L.; Wen, P.-C.; Thangapandian, S.; Tajkhorshid, E. The cellular membrane as a mediator for small molecule interaction with membrane proteins. *Biochim. Biophys. Acta - Biomembr.* **2016**, *1858*, 2290–2304, DOI: 10.1016/j.bbamem.2016.04.016.

(14) Sun, C.; Taguchi, A. T.; Vermaas, J. V.; Beal, N. J.; O'Malley, P. J.; Tajkhorshid, E.; Gennis, R. B.; Dikanov, S. A. Q-Band Electron-Nuclear Double Resonance Reveals Out-of-Plane Hydrogen Bonds Stabilize an Anionic Ubisemiquinone in Cytochrome bo_3 from *Escherichia coli*. *Biochemistry* **2016**, *55*, 5714–5725, DOI: 10.1021/acs.biochem.6b00669.

(15) Baylon, J. L.; Vermaas, J. V.; Muller, M. P.; Arcario, M. J.; Pogorelov, T. V.; Tajkhorshid, E. Atomic-level description of protein–lipid interactions using an accelerated membrane model. *Biochim. Biophys. Acta - Biomembr.* **2016**, *1858*, 1573–1583, DOI: 10.1016/j.bbamem.2016.02.027.

(16) Vermaas, J. V.; Hardy, D. J.; Stone, J. E.; Tajkhorshid, E.; Kohlmeyer, A. TopoGromacs: Automated Topology Conversion from CHARMM to GROMACS within VMD. *J. Chem. Inf. Model.* **2016**, *56*, 1112–1116, DOI: 10.1021/acs.jcim.6b00103.

(17) Trebesch, N.; Vermaas, J. V.; Tajkhorshid, E. In *Comput. Biophys. Membr. Proteins*, Domene, C., Ed.; Royal Society of Chemistry: Cambridge, 2016; Chapter 7, pp 197–236, DOI: 10.1039/9781782626695-00197.

(18) Vermaas, J.; Trebesch, N.; Mayne, C.; Thangapandian, S.; Shekhar, M.; Mahinthichaichan, P.; Baylon, J.; Jiang, T.; Wang, Y.; Muller, M.; Shinn, E.; Zhao, Z.; Wen, P.-C.; Tajkhorshid, E. In *Methods Enzymol.* 2016, pp 373–428, DOI: 10.1016/bs.mie.2016.05.042.

(19) Vermaas, J. V.; Petridis, L.; Qi, X.; Schulz, R.; Lindner, B.; Smith, J. C. Mechanism of lignin inhibition of enzymatic biomass deconstruction. *Biotechnol. Biofuels* **2015**, *8*, 217, DOI: 10.1186/s13068-015-0379-8.

(20) Qi, Y.; Cheng, X.; Lee, J.; Vermaas, J. V.; Pogorelov, T. V.; Tajkhorshid, E.; Park, S.; Klauda, J. B.; Im, W. CHARMM-GUI HMMM Builder for Membrane Simulations with the Highly Mobile Membrane-Mimetic Model. *Biophys. J.* **2015**, *109*, 2012–2022, DOI: 10.1016/j.bpj.2015.10.008.

(21) Vermaas, J. V.; Baylon, J. L.; Arcario, M. J.; Muller, M. P.; Wu, Z.; Pogorelov, T. V.; Tajkhorshid, E. Efficient Exploration of Membrane-Associated Phenomena at Atomic Resolution. *J. Membr. Biol.* **2015**, *248*, 563–582, DOI: 10.1007/s00232-015-9806-9.

(22) Vermaas, J. V.; Crowley, M. F.; Beckham, G. T.; Payne, C. M. Effects of Lytic Polysaccharide Monooxygenase Oxidation on Cellulose Structure and Binding of Oxidized Cellulose Oligomers to Cellulases. *J. Phys. Chem. B* **2015**, *119*, 6129–6143, DOI: 10.1021/acs.jpcb.5b00778.

(23) Vermaas, J. V.; Taguchi, A. T.; Dikanov, S. A.; Wraight, C. A.; Tajkhorshid, E. Redox Potential Tuning through Differential Quinone Binding in the Photosynthetic Reaction Center of Rhodobacter sphaeroides. *Biochemistry* **2015**, *54*, 2104–2116, DOI: 10.1021/acs.biochem.5b00033.

(24) Vermaas, J. V.; Tajkhorshid, E. Conformational heterogeneity of α -synuclein in membrane. *Biochim. Biophys. Acta - Biomembr.* **2014**, *1838*, 3107–3117, DOI: 10.1016/j.bbamem.2014.08.012.

(25) Pogorelov, T. V.; Vermaas, J. V.; Arcario, M. J.; Tajkhorshid, E. Partitioning of Amino Acids into a Model Membrane: Capturing the Interface. *J. Phys. Chem. B* **2014**, *118*, 1481–1492, DOI: 10.1021/jp4089113.

(26) Vermaas, J. V.; Tajkhorshid, E. A Microscopic View of Phospholipid Insertion into Biological Membranes. *J. Phys. Chem. B* **2014**, *118*, 1754–1764, DOI: 10.1021/jp409854w.

(27) Chamberlin, R. V.; Vermaas, J. V.; Wolf, G. H. Beyond the Boltzmann factor for corrections to scaling in ferromagnetic materials and critical fluids. *Eur. Phys. J. B* **2009**, *71*, 1–6, DOI: 10.1140/epjb/e2009-00278-0.

Conference Presentations (Past 3 years only)

2019 Dissocation Mechanism of Processive Cellulases Explored through Molecular Simulation **Oral Presentation** *ACS Fall 2019 National Meeting* San Diego, CA

2019 Molecular Interactions at the Cellulose-Lignin Interface Explored via Molecular Simulation **Oral Presentation** *ACS Fall 2019 National Meeting* San Diego, CA

2019 Electrostatic Lock Controlling Structural Transition in the EmrE Polyaromatic Cation Transporter **Oral Presentation** *Biophysical Society 63rd Annual Meeting* Baltimore, MD

2019 Binding Affinity Dependence of Lignin-Cellulose Complexes on Cellulose Faces and Lignin Composition *Biophysical Society 63rd Annual Meeting* Baltimore, MD

2019 Electrostatic Lock Controlling Structural Transition in the EmrE Polyaromatic Cation Transporter *Biophysical Society 63rd Annual Meeting* Baltimore, MD

2018 Binding Affinity Dependence of Lignin-Cellulose Complexes on Cellulose Faces and Lignin Composition **Oral Presentation** *256th ACS National Meeting* Boston, MA

2018 Membrane Binding of Soluble Enzymes, Explored Through Simulation of Bacterial P450s **Oral Presentation** *256th ACS National Meeting* Boston, MA

2018 Determining Differential Lignin Solvation and Structural Changes within Industrial Solvents *256th ACS National Meeting* Boston, MA

2018 Determining Differential Lignin Solvation and Structural Changes within Industrial Solvents *Lignin Gordon Research Conference* Easton, MA

2018 Computational Insights into Fuels and Chemicals Extraction from Microbial Biorefineries **Oral Presentation** *255th ACS National Meeting* New Orleans, LA

2018 Development Progress in Constructing Atomic Scale Models of Diverse Lignins **Oral Presentation** *255th ACS National Meeting* New Orleans, LA

2018 Computational Insights into Fuels and Chemicals Extraction from Microbial Biorefineries *Biophysical Society 62nd Annual Meeting* San Francisco, CA

2017 Development Progress in Constructing Atomic Scale Models of Diverse Lignins **Oral Presentation** *2017 MRS Fall Meeting and Exhibit* Boston, MA

2017 Cell-scale computational modeling methodologies for living membranes **Oral Presentation** *253rd ACS National Meeting* San Francisco, CA

2017 Systematic Parameterization of Lignin for the CHARMM Force Field *253rd ACS National Meeting* San Francisco, CA

2017 Systematic Parameterization of Lignin for the CHARMM Force Field *Biophysical Society 61st Annual Meeting* New Orleans, LA