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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

2021-Present **Assistant Professor**, *Michigan State University*, East Lansing, MI
Assistant professor in the plant research laboratory, using molecular simulation tools to study photosynthetic systems to deliver renewable energy and sustainable bioproducts.[4] Our laboratory develops tools to facilitate this research.[1,5] We are also active in collaborative Cryo-EM projects,[7,9] and other diverse molecular systems.[6]

2020–2020 **Computational Scientist**, *Oak Ridge Laboratory*, Oak Ridge, TN
INCITE liaison for NAMD-related projects,[14] and ensuring application readiness for NAMD on upcoming supercomputing systems. Also contributed to developing an accelerated drug-discovery pipeline for COVID-19 research.[10–13,16]

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,[15,19–21,23,25] membrane permeability,[3,21,26,28] and enzyme structure and mechanism.[22,24]

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[8,29,33,38,43] and application[30,42,44] of accelerated and conventional[30,31,35,36] membrane models, adding capabilities to the molecular dynamics visualization program VMD,[34] and simulations related to interactions within the photosynthetic reaction center of *Rhodobacter sphaeroides*[41] or cytochrome bo_3.[32]

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.[27]

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.[37]

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.[40] Supervised by Gregg Beckham, Michael Crowley, and Christina Payne. This was the foundation work for more recent studies for how oxidation changes cellulose crystallinity.[2]

2007-2010 **Undergraduate Researcher**, *Arizona State University*, Tempe, AZ

Diverse projects across the physics department to gague my interests across research fields and techniques,[45] 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.

Current Research Support

2022- Anton2 compute allocation

2022- NERSC compute allocation: m3968

2021- ACCESS allocation: TG-BIO210061

2021-2023 DOE BES: DE-FG02-91ER20021

2022-2024 DOE EFRC

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

2022 NAMD application judge and mentor for the Student Cluster Competition associated with the SuperComputing conference

2021 Nationwide Science Bowl volunteer

2020- Reviewer for XSEDE supercomputing allocations

2020 Moderator for Tennessee Science Bowl

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- Reviewer for several ACS, RSC, Cell Press, Springer and MDPI journals

Publications

(1) Sarkar, D.; Kulke, M.; Vermaas, J. V. LongBondEliminator: A Molecular Simulation Tool to Remove Ring Penetrations in Biomolecular Simulation Systems. *Biomolecules* **2023**, *13*, 107, DOI: 10.3390/biom13010107.

(2) Uchiyama, T.; Uchihashi, T.; Ishida, T.; Nakamura, A.; Vermaas, J. V.; Crowley, M. F.; Samejima, M.; Beckham, G. T.; Igarashi, K. Lytic Polysaccharide Monooxygenase Increases Cellobiohydrolases Activity by Promoting Decrystallization of Cellulose Surface. *Sci. Adv.* **2022**, *8*, eade5155, DOI: 10.1126/sciadv.ade5155.

(3) Vermaas, J. V.; Crowley, M. F.; Beckham, G. T. Molecular Simulation of Lignin-Related Aromatic Compound Permeation through Gram-Negative Bacterial Outer Membranes. *Journal of Biological Chemistry* **2022**, *298*, 102627, DOI: 10.1016/j.jbc.2022.102627.

(4) Andeme Ela, R. C.; Raza, S.; Heiden, P. A.; Vermaas, J. V.; Ong, R. G. Lignin Nanoparticle Morphology Depends on Polymer Properties and Solvent Composition: An Experimental and Computational Study. *ACS Appl. Polym. Mater.* **2022**, *4*, 6925–6935, DOI: 10.1021/acsapm.2c00854.

(5) Kulke, M.; Vermaas, J. V. Reversible Unwrapping Algorithm for Constant-Pressure Molecular Dynamics Simulations. *J. Chem. Theory Comput.* **2022**, *18*, 6161–6171, DOI: 10.1021/acs.jctc.2c00327.

(6) Ayala Mariscal, S. M.; Pigazzini, M. L.; Richter, Y.; Özel, M.; Grothaus, I. L.; Protze, J.; Ziege, K.; Kulke, M.; ElBediwi, M.; Vermaas, J. V.; Colombi Ciacchi, L.; Köppen, S.; Liu, F.; Kirstein, J. Identification of a HTT-specific Binding Motif in DNAJB1 Essential for Suppression and Disaggregation of HTT. *Nat Commun* **2022**, *13*, 4692, DOI: 10.1038/s41467-022-32370-5.

(7) Vant, J. W.; Sarkar, D.; Nguyen, J.; Baker, A. T.; Vermaas, J. V.; Singharoy, A. Exploring Cryo-Electron Microscopy with Molecular Dynamics. *Biochem. Soc. Trans.* **2022**, *50*, 569–581, DOI: 10.1042/BST20210485.

(8) Vermaas, J. V.; Mayne, C. G.; Shinn, E.; Tajkhorshid, E. Assembly and Analysis of Cell-Scale Membrane Envelopes. *J. Chem. Inf. Model.* **2022**, *62*, 602–617, DOI: 10.1021/acs.jcim.1c01050.

(9) Baker, A. T.; Boyd, R. J.; Sarkar, D.; Teijeira-Crespo, A.; Chan, C. K.; Bates, E.; Waraich, K.; Vant, J.; Wilson, E.; Truong, C. D.; Lipka-Lloyd, M.; Fromme, P.; Vermaas, J.; Williams, D.; Machiesky, L.; Heurich, M.; Nagalo, B. M.; Coughlan, L.; Umlauf, S.; Chiu, P.-L.; Rizkallah, P. J.; Cohen, T. S.; Parker, A. L.; Singharoy, A.; Borad, M. J. ChAdOx1 Interacts with CAR and PF4 with Implications for Thrombosis with Thrombocytopenia Syndrome. *Sci. Adv.* **2021**, *7*, eabl8213, DOI: 10.1126/sciadv.abl8213.

(10) Glaser, J.; Vermaas, J. V.; Rogers, D. M.; Larkin, J.; LeGrand, S.; Boehm, S.; Baker, M. B.; Scheinberg, A.; Tillack, A. F.; Thavappiragasam, M.; Sedova, A.; Hernandez, O. High-Throughput Virtual Laboratory for Drug Discovery Using Massive Datasets. *The International Journal of High Performance Computing Applications* **2021**, *35*, 452–468, DOI: 10.1177/10943420211001565.

(11) Vermaas, J. V.; Sedova, A.; Baker, M.; Boehm, S.; Rogers, D.; Larkin, J.; Glaser, J.; Smith, M.; Hernandez, O.; Smith, J. Supercomputing Pipelines Search for Therapeutics Against COVID-19. *Comput. Sci. Eng.* **2021**, *23*, 7–16, DOI: 10.1109/MCSE.2020.3036540.

(12) Pavlova, A.; Lynch, D. L.; Daidone, I.; Zanetti-Polzi, L.; Smith, M. D.; Chipot, C.; Kneller, D. W.; Kovalevsky, A.; Coates, L.; Golosov, A. A.; Dickson, C. J.; Velez-Vega, C.; Duca, J. S.; Vermaas, J. V.; Pang, Y. T.; Acharya, A.; Parks, J. M.; Smith, J. C.; Gumbart, J. C. Inhibitor Binding Influences the Protonation States of Histidines in SARS-CoV-2 Main Protease. *Chem. Sci.* **2021**, *12*, 1513–1527, DOI: 10.1039/D0SC04942E.

(13) Acharya, A.; Agarwal, R.; Baker, M. B.; Baudry, J.; Bhowmik, D.; Boehm, S.; Byler, K. G.; Chen, S. Y.; Coates, L.; Cooper, C. J.; Demerdash, O.; Daidone, I.; Eblen, J. D.; Ellingson, S.; Forli, S.; Glaser, J.; Gumbart, J. C.; Gunnels, J.; Hernandez, O.; Irle, S.; Kneller, D. W.; Kovalevsky, A.; Larkin, J.; Lawrence, T. J.; LeGrand, S.; Liu, S.-H.; Mitchell, J.; Park, G.; Parks, J.; Pavlova, A.; Petridis, L.; Poole, D.; Pouchard, L.; Ramanathan, A.; Rogers, D. M.; Santos-Martins, D.; Scheinberg, A.; Sedova, A.; Shen, Y.; Smith, J. C.; Smith, M. D.; Soto, C.; Tsaris, A.; Thavappiragasam, M.; Tillack, A. F.; Vermaas, J. V.; Vuong, V. Q.; Yin, J.; Yoo, S.; Zahran, M.; Zanetti-Polzi, L. Supercomputer-Based Ensemble Docking Drug Discovery Pipeline with Application to COVID-19. *J. Chem. Inf. Model.* **2020**, *60*, 5832–5852, DOI: 10.1021/acs.jcim.0c01010.

(14) Vant, J. W.; Sarkar, D.; Streitwieser, E.; Fiorin, G.; Skeel, R.; Vermaas, J. V.; Singharoy, A. Data-Guided Multi-Map Variables for Ensemble Refinement of Molecular Movies. *J. Chem. Phys.* **2020**, *153*, 214102, DOI: 10.1063/5.0022433.

(15) Vermaas, J. V.; Crowley, M. F.; Beckham, G. T. Molecular Lignin Solubility and Structure in Organic Solvents. *ACS Sustain. Chem. Eng.* **2020**, *8*, 17839–17850, DOI: 10.1021/acssuschemeng.0c07156.

(16) LeGrand, S.; Scheinberg, A.; Tillack, A. F.; Thavappiragasam, M.; Vermaas, J. V.; Agarwal, R.; Larkin, J.; Poole, D.; Santos-Martins, D.; Solis-Vasquez, L.; Koch, A.; Forli, S.; Hernandez, O.; Smith, J. C.; Sedova, A. In *Proc. 11th ACM Int. Conf. Bioinforma. Comput. Biol. Health Inform.* ACM: New York, NY, USA, 2020, pp 1–10, DOI: 10.1145/3388440.3412472.

(17) Thornburg, N. E.; Pecha, M. B.; Brandner, D. G.; Reed, M. L.; Vermaas, J. V.; Michener, W. E.; Katahira, R.; Vinzant, T. B.; Foust, T. D.; Donohoe, B. S.; Román-Leshkov, Y.; Ciesielski, P. N.; Beckham, G. T. Mesoscale Reaction–Diffusion Phenomena Governing Lignin-First Biomass Fractionation. *ChemSusChem* **2020**, *13*, 4495–4509, DOI: 10.1002/cssc.202000558.

(18) Ciesielski, P. N.; Pecha, M. B.; Lattanzi, A. M.; Bharadwaj, V. S.; Crowley, M. F.; Bu, L.; Vermaas, J. V.; Steirer, K. X.; Crowley, M. F. Advances in Multiscale Modeling of Lignocellulosic Biomass. *ACS Sustain. Chem. Eng.* **2020**, *8*, 3512–3531, DOI: 10.1021/acssuschemeng.9b07415.

(19) Vermaas, J. V.; Crowley, M. F.; Beckham, G. T. A Quantitative Molecular Atlas for Interactions Between Lignin and Cellulose. *ACS Sustainable Chem. Eng.* **2019**, *7*, 19570–19583, DOI: 10.1021/acssuschemeng.9b04648.

(20) 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 Sustainable Chem. Eng.* **2019**, *7*, 18313–18322, DOI: 10.1021/acssuschemeng.9b03534.

(21) 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. U. S. A.* **2019**, *116*, 23117–23123, DOI: 10.1073/pnas.1904643116.

(22) 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. U. S. A.* **2019**, *116*, 23061–23067, DOI: 10.1073/pnas.1913398116.

(23) 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.

(24) Zheng, F.; Vermaas, J. V.; Zheng, J.; Wang, Y.; Tu, T.; Wang, X.; Xie, X.; Yao, B.; Beckham, G. T.; Luo, H. Characterizing 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.

(25) 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.

(26) 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.

(27) Vermaas, J. V.; Rempe, S. B.; Tajkhorshid, E. Electrostatic Lock in the Transport Cycle of the Multidrug Resistance Transporter EmrE. *Proc. Natl. Acad. Sci. U. S. A.* **2018**, *115*, E7502–E7511, DOI: 10.1073/pnas.1722399115.

(28) 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.

(29) 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.

(30) 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.

(31) 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 BBA - Biomembr.* **2016**, *1858*, 2290–2304, DOI: 10.1016/j.bbamem.2016.04.016.

(32) 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<inf>3</Inf> from *Escherichia Coli*. *Biochemistry* **2016**, *55*, 5714–5725, DOI: 10.1021/acs.biochem.6b00669.

(33) 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 BBA - Biomembr.* **2016**, *1858*, 1573–1583, DOI: 10.1016/j.bbamem.2016.02.027.

(34) 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.

(35) Trebesch, N.; Vermaas, J. V.; Tajkhorshid, E. In *Theoretical and Computational Chemistry Series*, Domene, C., Ed.; Royal Society of Chemistry: Cambridge, 2016, pp 197–236, DOI: 10.1039/9781782626695-00197.

(36) 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 in Enzymology*; Elsevier: 2016; Vol. 578, pp 373–428, DOI: 10.1016/bs.mie.2016.05.042.

(37) 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.

(38) 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.

(39) 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.

(40) 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.

(41) 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.

(42) Vermaas, J. V.; Tajkhorshid, E. Conformational Heterogeneity of α-Synuclein in Membrane. *Biochim. Biophys. Acta BBA - Biomembr.* **2014**, *1838*, 3107–3117, DOI: 10.1016/j.bbamem.2014.08.012.

(43) 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.

(44) 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.

(45) 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.

Invited Presentations

2022 Tracking Carbon Diffusion in Photosynthesis from a Molecular Perspective, *Biophysics Seminar Series* Arizona State University

2022 Tracking Carbon Diffusion in Photosynthesis from a Molecular Perspective, National Renewable Energy Laboratory

2021 Exploring biological mechanisms and materials through molecular simulation for a sustainable bioeconomy *School of Molecular Sciences Seminar* Arizona State University

2021 Exploring biological mechanisms and materials to enable the bioeconomy through computational physics *Theoretical and Computational Biophysics Group Seminar* University of Illinois at Urbana-Champaign

Conference Presentations (Past 3 years only)

2022 Quantifying temperature dependent mesophyll conductance within leaf plasma membranes **Oral Presentation** *ACS Fall 2022 National Meeting* Chicago, IL

2022 Predicting Lignin Depolymerization Pathways and Products at High Temperature through Molecular Dynamics Simulation *Lignin Gordon Conference* Easton, MA

2022 Exploring Lignin Interactions Within the Cell Wall Through Computational Microscopy **Oral Presentation** *IX Cell Wall Research Conference* East Lansing, MI

2022 Tracking Photosynthetic Reactant and Product Diffusion Across Cyanobacterial Carboxysomes on Exascale Computing Platforms **Oral Presentation** *Biophysics at the Dawn to Exascale Computing* Hamburg, Germany

2022 Measuring heme-hopping electron transfer through a biological nanowire *Biophysical Society 66th Annual Meeting* San Francisco, CA

2021 Quantifying solvent impacts on lignin-cellulose interactions in diverse solvents **Oral Presentation** *ACS Fall 2021 National Meeting* Virtual Meeting

2021 Comparing inner and outer membrane permeabilities for lignin related aromatic compounds in a biorefinery context **Oral Presentation** *ACS Spring 2021 National Meeting* Virtual Meeting

2021 Exploring solvent-dependence in lignin polymer shape and structure through molecular simulation **Oral Presentation** *ACS Spring 2021 National Meeting* Virtual Meeting

2021 Comparing Inner and Outer Membrane Permeabilities for Lignin Related Aromatic Compounds *Biophysical Society 65th Annual Meeting* Virtual Meeting

2020 High-Throughput Virtual Laboratory for Drug Discovery Using Massive Datasets **Oral Presentation** *SC20* Virtual Meeting

2020 Dissociation Mechanism of Processive Cellulases Explored through Molecular Simulation
Biophysical Society 64th Annual Meeting San Diego, CA