

# CHRISTINA M. PAYNE, PE, PhD

National Science Foundation  
Chemical, Bioengineering, Environmental and Transport Systems  
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## EDUCATION

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2002 - 2007 Ph.D., Chemical Engineering, Vanderbilt University  
1998 - 2002 B.S., Chemical Engineering, *summa cum laude*, Tennessee Technological University

## PROFESSIONAL & RESEARCH EXPERIENCE

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2018 - present Program Director, *Interfacial Engineering*, National Science Foundation (NSF)  
2017 - present Adjunct Professor, Chemical and Materials Engineering Dept., University of Kentucky  
2018 Acting Program Director, *Engineering of Biomedical Systems and Disability and Rehabilitation Engineering*, National Science Foundation  
2017 - 2018 Associate Program Director, *Engineering Biology and Health*, National Science Foundation  
2012 - 2017 Assistant Professor, Chemical and Materials Engineering Dept., University of Kentucky  
(Promoted to Associate Professor with tenure, May 2017)  
2013 - 2017 August T. Larsson Guest Researcher, Swedish University of Agricultural Sciences  
2011 - 2012 Staff Scientist, National Renewable Energy Laboratory  
2011 Postdoctoral Research Associate, National Renewable Energy Laboratory  
2008 - 2011 Chemical Process Engineer, URS (acquired by AECOM)  
2002 - 2007 Research Assistant, Vanderbilt University (Advisor: Peter T. Cummings)  
2005 DOE Computational Science Graduate Fellow, Sandia National Laboratory  
2000 Engineering Intern, DuPont, Old Hickory, TN

## HONORS & AWARDS

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2022 NSF Special Act Award – *In recognition of role in supporting NSF's participation in the Interagency Marine Debris Coordinating Committee*  
2021 NSF Special Act Award - *In recognition of excellent leadership of NSF's efforts on the end-of-life plastics environmental problem*  
2021 NSF Special Act Award - *In recognition of excellent leadership of special program, Environmental Convergence Opportunities in CBET (ECO-CBET)*  
2020 NSF Special Act Award - *In recognition of outstanding leadership in developing the ECO-CBET Program that provides support to teams of researchers to study grand challenge problems that integrate environmental engineering and sustainability with process sciences*  
2019 NSF Special Act Award - *For outstanding achievement of envisioning, successfully pitching, and building partnerships for her proposal for the Emerging Frontiers in Research and Innovation solicitation on topic of "Engineering the Elimination of End-of-Life Plastics"*  
2019 Presidential Early Career Award for Scientists and Engineers (PECASE)  
2017 University of Kentucky College of Engineering Dean's Award for Excellence in Research  
2016 NSF CAREER Award

2014	ORAU Ralph E. Powe Junior Faculty Award
2013	NSF Bioinformatics Workshop, First Place – Faculty Division – Poster Award
2012	Professional Engineer, #28848, KY State
2012	Professional Engineer, #46559, CO State
2010	Induction into URS Top Talent Program
2006	Vanderbilt Institute of Nanoscale Science and Engineering (VINSE) Nanoday Poster Contest, First Place
2003 - 2007	Department of Energy Computational Science Graduate Fellowship (DOE CSGF)
2002 - 2006	IBM Fellowship

#### PATENTS & PATENT APPLICATIONS

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1. E. M. Erickson, G. T. Beckham, J. E. Gado, J. E. McGeehan, **C. M. Payne** (2022). Polymer Degrading Enzymes. U.S. Patent Application No. PCT/US2022/025624 (WO/2022/226109), filed April 20, 2022.

#### REFEREED PUBLICATIONS

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\*Corresponding

†Equally contributing

1. A. Mariotti\*, E. Nichols\*, K. Beers, K. Cochrane, J. Cresko, E. Golan, H. Ho, A. Kreps, L. K. Molnar, **C. M. Payne**, and A. Stephens, "Accelerating U.S. circular economy innovation: benefits and opportunities," *in preparation*.
2. T. Haataja, J. E. Gado, A. Nutt, N. Anderson, M. Nilsson, M. H. Momeni, R. Isaksson, P. Väljamäe, G. Johansson\*, **C. M. Payne\***, and J. Ståhlberg\*, "Enzyme kinetics by GH7 cellobiohydrolases on chromogenic substrates are dictated by non-productive binding: insights from crystal structures and molecular dynamics simulation," *FEBS J.*, **290(2)**, 379-399 (2023) [DOI: 10.1111/febs.16602].
3. E. Erickson†, J. E. Gado†, L. Avilan, F. Bratti, R. K. Brizendine, P. A. Cox, R. Gill, R. Graham, D. Kim, G. König, W. E. Michener, S. Poudel, K. J. Ramirez, T. J. Shakespeare, M. Zahn, E. S. Boyd, **C. M. Payne**, J. L. DuBois, A. R. Pickford, G. T. Beckham\*, and J. E. McGeehan\*, "Sourcing thermotolerant poly(ethylene terephthalate) hydrolase scaffolds from natural diversity," *Nat. Commun.*, **13(1)**, 7850 (2022).
4. J. M. Herbert\*, M. Head-Gordon, H. P. Hratchian, T. Head-Gordon, R. E. Amaro, A. Aspuru-Guzik, R. Hoffmann, C. A. Parish, **C. M. Payne**, and T. Van Voorhis, "Words matter: On the debate over free speech, inclusivity, and academic excellence," *J. Phys. Chem. Lett.*, **13(30)**, 7100-7104 (2022).
5. J. E. Gado, B. E. Harrison, M. Sandgren, J. Ståhlberg, G. T. Beckham\*, and **C. M. Payne\***, "Machine learning reveals sequence-function relationships in family 7 glycoside hydrolases," *J. Biol. Chem.* **297(2)**, 100931 (2021). [bioRxiv, DOI: 10.1101/2020.11.06.372003].
6. B. C. Knott†, E. Erickson†, M. D. Allen†, J. E. Gado†, R. Graham, F. L. Kearns, I. Pardo, E. Topuzlu, J. J. Anderson, H. P. Austin, G. Dominick, C. W. Johnson, N. A. Rorrer, C. J. Szostkiewicz, V. Copié, **C. M. Payne**, H. L. Woodcock, B. S. Donohoe, G. T. Beckham\*, and J. E. McGeehan\*, "Characterization and engineering of a two-enzyme system for plastics depolymerization," *Proc. Natl. Acad. Sci. U.S.A.*, **117(41)**, 25476-25485 (2020).
7. J. E. Gado, G. T. Beckham\*, and **C. M. Payne\***, "Improving enzyme optimum temperature prediction with resampling strategies and ensemble learning," *J. Chem. Inf. Model.*, **60(8)**, 4098-4107 (2020) [bioRxiv, DOI: 10.1101/2020.05.06.081737].

8. Y. Yue<sup>‡</sup>, L. C. Mills<sup>‡</sup>, D. L. Englert, and **C. M. Payne\***, "Inhibition mechanisms of *Rhodococcus erythropolis* 2'-hydroxybiphenyl-2-sulfinate desulfinate (DszB)," *J. Phys. Chem. B.*, **12(43)**, 9054-9065 (2019).
9. S. Jana<sup>‡</sup>, A. G. Hamre<sup>‡</sup>, V. G. H. Eijsink, M. Sørlie\*, and **C. M. Payne\***, "Polar residues lining the binding cleft of a *Serratia marcescens* Family 18 chitinase position the substrate for attack and stabilize associative interactions," *Mol. Phys.*, **117 (23-24)**, 3664-3682 (2019).
10. M. M. Machovina<sup>‡</sup>, S. J. B. Mallinson<sup>‡</sup>, B. C. Knott<sup>‡</sup>, A. W. Meyers<sup>‡</sup>, M. Garcia-Borràs<sup>‡</sup>, L. Bu, J. E. Gado, A. Oliver, G. P. Schmidt, D. J. Hinchin, M. F. Crowley, C. W. Johnson, E. L. Neidle, **C. M. Payne**, K. N. Houk\*, G. T. Beckham\*, J. E. McGeehan\*, J. L. DuBois\*, "Enabling microbial syringol conversion through structure-guided protein engineering," *Proc. Natl. Acad. Sci. U.S.A.*, **116 (28)**, 13970-13976 (2019).
11. A. G. Hamre, A. Kaupang, **C. M. Payne**, P. Väljamäe, and M. Sørlie\*, "Thermodynamics signatures of substrate binding for three *Thermobifida fusca* cellulases with different modes of action," *Biochemistry*, **58:12**, 1648-1659 (2019).
12. I. Geronimo, P. Ntarima, K. Piens, M. Gudmundsson, H. Hansson, M. Sandgren\*, and **C. M. Payne\***, "Kinetic and molecular dynamics study of inhibition and transglycosylation in *Hypocrea jecorina* family 3  $\beta$ -glucosidases," *J. Biol. Chem.*, **294**, 3169-3180 (2019).
13. A. A. Kognole and **C. M. Payne\***, "Cellulose-specific Type B carbohydrate binding modules: understanding oligomeric and non-crystalline recognition mechanisms," *Biotech. Biofuels*, **11:319** (2018).
14. I. Geronimo, **C. M. Payne\***, and M. Sandgren\*, "Hydrolysis and transglycosylation transition states of glycoside hydrolase Family 3  $\beta$ -glucosidases differ in charge and puckering conformation," *J. Phys. Chem. B*, **122(41)**, 9452-9459 (2018).
15. I. Geronimo, C. A. Denning, D. K. Heidary, E. C. Glazer\*, and **C. M. Payne\***, "Molecular determinants of substrate affinity and enzyme activity of a cytochrome P450<sub>BM3</sub> variant," *Biophys. J.*, **115(7)**, 1251-1263 (2018).
16. B. Liu, A. A. Kognole, M. Wu, B. Westereng, M. F. Crowley, S. Kim, M. Dimarogona\*, **C. M. Payne\***, M. Sandgren\*, "Structural and molecular dynamics studies of a C1-oxidizing lytic polysaccharide monooxygenase from *Heterobasidion irregulare* reveal amino acids important for substrate recognition," *FEBS J.*, **285**, 2225-2242 (2018).
17. I. Geronimo, **C. M. Payne**, and M. Sandgren\*, "The role of catalytic residue pK<sub>a</sub> on the hydrolysis/transglycosylation partition in family 3  $\beta$ -glucosidases," *Org. Biomol. Chem.*, **16**, 316-324 (2018).
18. A. S. Borisova, E. V. Eneyskaya, S. Jana, S. F. Badino, J. Kari, A. Amore, M. Karlsson, H. Hansson, M. Sandgren, M. E. Himmel, P. Westh, **C. M. Payne\***, A. A. Kulminskaya\*, and J. Stahlberg\*, "Correlation of structure, function and protein dynamics in GH7 cellobiohydrolases from *Trichoderma atroviride*, *T. reesei* and *T. harzianum*," *Biotech. Biofuels*, **11:5** (2018).
19. F. Goedegebuur\*, L. Dankmeyer, P. Gualfetti, S. Karkehabadi, H. Hansson, S. Jana, V. Huynh, B. R. Kelemen, P. Kruihof, E. A. Larenas, P. J. M. Teunissen, J. Ståhlberg, **C. M. Payne\***, C. Mitchinson, and M. Sandgren\*, "Improving the thermal stability of cellobiohydrolase Cel7A from *Hypocrea jecorina* by directed evolution," *J. Biol. Chem.*, **42**, 17418-17430 (2017).
20. I. Geronimo, S. Nigam, and **C. M. Payne\***, "Desulfination by 2'-hydroxybiphenyl-2-sulfinate desulfinate proceeds via electrophilic aromatic substitution by the Cys27 proton," *Chem. Sci.*, **8**, 5078-5086 (2017).
21. A. A. Kognole and **C. M. Payne\***, "Inhibition of mammalian glycoprotein YKL-40: Identification of the physiological ligand," *J. Biol. Chem.*, **292(7)**, 2624-2636 (2017).

22. Y. Yu, I. Fursule, L. C. Mills, D. L. Englert, B. J. Berron, and **C. M. Payne\***, "CHARMM force field parameters for 2'-hydroxybiphenyl-2-sulfinate, 2-hydroxybiphenyl, and related analogs," *J. Mol. Graphics Modell.*, **72**, 32-42 (2017).
23. I. Geronimo, C. A. Denning, W. E. Rogers, T. Othman, T. Huxford, D. K. Heidary, E. C. Glazer\*, and **C. M. Payne\***, "Effect of mutation and substrate binding on the stability of cytochrome P450<sub>BM3</sub> variants," *Biochemistry*, **55(25)**, 3594-3606 (2016).
24. S. Jana<sup>‡</sup>, A. G. Hamre<sup>‡</sup>, P. Wildberger, M. M. Holen, V. G. H. Eijsink, G. T. Beckham, M. Sørlie\*, and **C. M. Payne\***, "Aromatic-mediated carbohydrate recognition in processive *Serratia marcescens* chitinases," *J. Phys. Chem. B*, **120(7)**, 1236-1249 (2016).
25. C. Wilkens<sup>‡</sup>, K. Auger<sup>‡</sup>, N. T. Anderson, D. A. Meekins, M. Raththagala, M. A. Hachem, **C. M. Payne**, M. S. Gentry\*, and B. Svensson\*, "Plant  $\alpha$ -glucan phosphatases SEX4 and LSF2 display different affinity for amylopectin and amylose," *FEBS Lett.*, **590(1)**, 118-128 (2016).
26. A. G. Hamre<sup>‡</sup>, S. Jana<sup>‡</sup>, N. K. Reppert, **C. M. Payne\***, and M.S. Sørlie\*, "Processivity, substrate positioning and binding: The role of polar residues in a family 18 glycoside hydrolase," *Biochemistry*, **119(30)**, 9601-9613 (2015).
27. A. S. Borisova, E. V. Eneyskaya, K. S. Bobrov, S. Jana, A. Logachev, D. E. Poley, A. L. Lapidus, F. Ibatullin, M. Sandgren, **C. M. Payne\***, A. A. Kulminskaya\*, and J. Ståhlberg\*, "Sequencing, biochemical characterization, crystal structure, and molecular dynamics of cellobiohydrolase Cel7A from *Geotrichum candidum*," *FEBS J.*, **282(23)**, 4515-4537 (2015).
28. A. Borisova, T. Isaksen, M. Dimarogona, A. A. Kognole, G. Mathiesen, A. Várnai, Å. Røhr, **C. M. Payne**, M. Sørlie, M. Sandgren, and V. G. H. Eijsink\*, "Structural and functional characterization of a lytic polysaccharide monooxygenase with broad substrate specificity," *J. Biol. Chem.*, **290(38)**, 22955-22969 (2015).
29. A. G. Hamre<sup>‡</sup>, S. Jana<sup>‡</sup>, M. M. Holen, G. Mathiesen, P. Väljamäe, **C. M. Payne\***, and M.S. Sørlie\*, "Thermodynamic relationships with processivity in *Serratia marcescens* family 18 chitinases," *J. Phys. Chem. B*, **119(30)**, 9601-9613 (2015).
30. A. A. Kognole and **C. M. Payne\***, "Ligand binding dynamics and directionality in *Cellulomonas fimi* Family 4 carbohydrate binding modules," *Glycobiology*, **25(10)**, 1100-1111 (2015).
31. J. V. Vermaas, M. F. Crowley, G. T. Beckham, and **C. M. Payne\***, "Effects of lytic polysaccharide monooxygenase oxidation on cellulose structure and binding of oxidized cellulose oligomers to cellulases," *J. Phys. Chem. B*, **119(20)**, 6129-6143 (2015).
32. **C. M. Payne\***, B.C. Knott<sup>‡</sup>, H. Mayes<sup>‡</sup>, H. Hansson, M. Sandgren, J. Ståhlberg, M.E. Himmel, and G. T. Beckham\*, "Fungal cellulases," *Chem. Rev.*, **115(3)**, 1308-1448 (2015).
33. G. T. Beckham\*, J. Ståhlberg\*, B.C. Knott, M.E. Himmel, M.F. Crowley, M. Sandgren, M. Sørlie, and **C. M. Payne\***, "Towards a molecular-level theory of carbohydrate processivity in glycoside hydrolases," *Curr. Opin. Biotechnol.*, **27**, 96-106 (2014).
34. **C. M. Payne\***<sup>‡</sup>, W. Jiang<sup>‡</sup>, M. R. Shirts, M. E. Himmel, M. F. Crowley, G. T. Beckham, "Glycoside hydrolase processivity is directly related to oligosaccharide binding free energy," *J. Am. Chem. Soc.*, **135(50)**, 18831-18839 (2013).
35. **C. M. Payne\***<sup>‡</sup>, M. G. Resch<sup>‡</sup>, L. Chen<sup>‡</sup>, M. F. Crowley, M. E. Himmel, L. E. Taylor, M. Sandgren, J. Ståhlberg, I. Stals\*, Z. Tan\*, and G. T. Beckham\*, "Glycosylated linkers in multi-modular lignocellulose degrading enzymes dynamically bind to cellulose," *Proc. Natl. Acad. Sci. U.S.A.*, **110**, 14646-14651 (2013).
36. M. Kern, J.E. McGeehan, S.D. Streeter, R. N. A. Martin, K. Besser, L. Elias, W. Eborral, G.P. Malyon, **C. M. Payne**, M. E. Himmel, K. Schnorr, G. T. Beckham\*, S. M. Cragg\*, N. C. Bruce\*, S.J. McQueen-Mason\*, "Structural characterization of a Family 7 cellobiohydrolase from a marine animal reveals potential mechanisms of cellulase salt tolerance," *Proc. Natl. Acad. Sci. U.S.A.*, **110**, 10189-10194 (2013).

37. R. Kushwaha, A. B. Downie, and **C. M. Payne\***, "Uses of phage display in agriculture: Sequence analysis and comparative modeling of late embryogenesis abundant client proteins suggests protein-nucleic acid binding functionality," *Comput. Math. Methods Med.*, **2013**, 470390 (2013).
38. R. Kushwaha, **C. M. Payne**, and A. B. Downie\*, "Uses of phage display in agriculture: A review of food-related protein-protein interactions discovered by biopanning over diverse baits," *Comput. Math. Methods Med.*, **2013**, 653759 (2013).
39. C. B. Taylor, **C. M. Payne**, M. E. Himmel, M. F. Crowley, C. McCabe, and G. T. Beckham\*, "Binding site dynamics and aromatic-carbohydrate interactions important for processivity in Family 7 cellulases," *J. Phys. Chem. B*, **117**, 4924-4933 (2013).
40. M. Wu, G. T. Beckham\*, A. M. Larsson, T. Ishida, S. Kim, **C. M. Payne**, M. E. Himmel, M. F. Crowley, S. J. Horn, B. Westereng, K. Igarashi, M. Samejima, J. Ståhlberg, V. G. H. Eijsink, M. Sandgren\*, "Crystal structure and computational characterization of the lytic polysaccharide monoxygenase GH61D from the basidiomycota fungus *Phanerochaete chrysosporium*," *J. Biol. Chem.*, **288**, 12828-12839 (2013).
41. M. H. Momeni<sup>‡</sup>, **C. M. Payne\***, H. Hansson, N. E. Mikkelsen, J. Svedberg, Å. Engström, M. Sandgren, G. T. Beckham\*, and J. Ståhlberg\*, "Structural, biochemical, and computational characterization of the glycoside hydrolase Family 7 cellobiohydrolase of the tree-killing fungus *Heterobasium irregulare*," *J. Biol. Chem.*, **288**, 5861-5872 (2013).
42. D. W. Sammond, **C. M. Payne**, R. Brunecky, M. E. Himmel, M. F. Crowley, and G. T. Beckham\*, "Cellulase linkers are optimized based on domain type and function: Insights from sequence analysis, biophysical measurements, and molecular simulation," *PLoS ONE*, **7**, e48615 (2012).
43. **C. M. Payne**, J. Baban, S. J. Horn, P. H. Backe, A. S. Arvai, B. Dalhus, M. Bjørås, V. G. H. Eijsink, M. Sørli, G. T. Beckham\*, and G. Vaaje-Kolstad\*, "Hallmarks of processivity in glycoside hydrolases from crystallographic and computational studies of the *Serratia marcescens* chitinases," *J. Biol. Chem.*, **287**, 36322-36330 (2012).
44. G. T. Beckham\*, Z. Dai, J. F. Matthews, M. Momany, **C. M. Payne**, W.S. Adney, S.E. Baker, and M.E. Himmel, "Harnessing glycosylation to improve cellulase activity," *Curr. Opin. Biotechnol.*, **23**, 338-345 (2012).
45. **C. M. Payne**, Y. J. Bomble, C. B. Taylor, C. McCabe, M. E. Himmel, M. F. Crowley, and G. T. Beckham\*, "Multiple functions of aromatic-carbohydrate interactions in a processive enzyme tunnel examined with molecular simulation," *J. Biol. Chem.*, **286**, 41028-41035 (2011).
46. **C. M. Payne\***, M. E. Himmel, M. F. Crowley, and G. T. Beckham, "Decrystallization of oligosaccharides from the cellulose 1 $\beta$  surface with molecular simulation," *J. Phys. Chem. Lett.*, **2**, 1546-1550 (2011).
47. B. K. Evans, A. Samadi, J. B. Mason, W. S. Roesener, **C. M. Payne**, and V. Vora, "Fluidized bed steam reforming production facility design for the conversion of Savannah River Tank 48 high-level waste into a soluble granular carbonate product," *Waste Management Symposia Proceedings* (2011).
48. **C. M. Payne**, B. K. Evans, J. B. Mason, A. Olson, K. Ryan and V. Vora, "Fluidized bed steam reforming technology demonstration for conversion of Savannah River Tank 48 waste to a granular carbonate product," *Waste Management Symposia Proceedings* (2010).
49. X. Zhao, **C. M. Payne**, and P. T. Cummings, "Controlled translocation of DNA segments through nanoelectrode gaps from molecular dynamics," *J. Phys. Chem. C*, **112**, 9-12 (2008).
50. **C. M. Payne**, X. Zhao, and P. T. Cummings, "Electrophoresis of ssDNA through nanoelectrode gaps from molecular dynamics: Impact of gap width and chain length," *J. Phys. Chem. B*, **112**, 12851-12858 (2008).
51. **C. M. Payne\***, X. Zhao, L. Vlcek, and P. T. Cummings, "Molecular dynamics simulation of ssDNA translocation between copper nanoelectrodes incorporating electrode charge dynamics," *J. Phys. Chem. B*, **112**, 1712-1717 (2008).

52. X. Zhao, **C. M. Payne**, P. T. Cummings, and J. W. Lee, "Single-strand DNA molecule translocation through nanoelectrode gaps," *Nanotechnology*, **18**, 424018 (2007).
53. **C. M. Payne\***, X. Zhao, and P. T. Cummings, "Molecular simulations of DNA transport in solution," *Molecular Simulation*, **33**, 399 – 403 (2007).
54. **C. M. Smith (née Payne)** and D. P. Visco, Jr., "Evaluating the thermodynamic consistency of experimental data for HF+H<sub>2</sub>O at 101.325 kPa," *J. Chem. Eng. Data*, **49**, 306 – 310 (2004).

## SPONSORED RESEARCH

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1. *Mechanisms of Biological and Chemical Catalysts in Plant Biomass Synthesis, Deconstruction, and Conversion to Fuel* (#TG-MCB090159)  
(resigned as PI due to employment with NSF); PI: Gregg T. Beckham  
**National Science Foundation XSEDE**; 10/17 – 09/18; Total: 25,976,591 SUs System Units (\$428,809)
2. *Mechanisms of Biological and Chemical Catalysts in Plant Biomass Synthesis, Deconstruction, and Conversion to Fuel* (#TG-MCB090159)  
PI; co-PI: Gregg T. Beckham  
**National Science Foundation XSEDE**; 10/16 – 09/17; Total: 13,146,680 System Units (\$754,946)
3. *MRI: Acquisition of the Kentucky Research Informatics Cloud* (ACI #1626364)  
**Co-PI**; PI: G. Q. Zhang (resigned as co-PI due to employment with NSF)  
**National Science Foundation – ACI**; 08/16 – 07/19; Total \$2,240,000 + \$960,000 UK cost share
4. *CAREER: Processivity and Substrate Binding in Glycoside Hydrolases* (CBET #1552355)  
PI (substitute PI – Thomas Dziubla)  
**National Science Foundation – CBET: Catalysis and Biocatalysis**; 05/16 – 04/22; Total: \$524,492
5. *Computational Studies of Biological and Chemical Systems* (#TG-MCB090159)  
**Co-PI**; PI: Gregg T. Beckham  
**National Science Foundation XSEDE**; 10/15 – 09/16; Total: 26,140,777 System Units (\$1,158,600)
6. *Computational Studies of Biological and Chemical Systems* (#TG-MCB090159)  
**Co-PI**; PI: Gregg T. Beckham  
**National Science Foundation XSEDE**; 10/14 – 09/15; Total: 17,500,000 System Units (\$856,350)
7. *Resolving Molecular Mechanisms of Biomass Degrading Enzymes Through a Combined Computational and Experimental Approach* (#240967)  
**Research Partner**; PI: Åsmund Kjendseth Røhr  
**Research Council of Norway**; 04/15 – 09/18; Total: 6,996,000 NOK (\$890,269)
8. *SusChEM: Carbohydrate Recognition in Type B Carbohydrate Binding Modules* (CHE #1404849)  
PI (substitute PI – Thomas Dziubla)  
**National Science Foundation – CHE: Chemistry for Life Processes**; 07/14 – 01/19; Total: \$225,000
9. *NSF EPSCoR: Powering the Kentucky Bioeconomy for a Sustainable Future* (#1355438)  
**Faculty Participant**; PI: Rodney Andrews  
**National Science Foundation**; 07/14 – 06/19; Total: \$24,000,000 (~\$300,000 to C. M. Payne)
10. *ORAU Ralph E. Powe Junior Faculty Enrichment Award* (FY2014\_419)  
PI  
**Oak Ridge Associated Universities (ORAU)**; 07/14 – 06/15; Total: \$10,000

11. *Understanding the Molecular Mechanism of Biological Desulfurization to Improve Sulfur Removal from Petroleum* (#23861-DNI4)  
**PI**  
**American Chemical Society Petroleum Research Fund**; 09/14 – 08/17; Total: \$100,000
12. *Developing the Foundation of Sequence-based Performance Prediction in Fungal Glycoside Hydrolases*  
**PI**; Hosts: Henrik Hansson and Jerry Ståhlberg  
**Swedish University of Agricultural Sciences**; 05/14 – 08/17; Total: \$195,000
13. *Computational Studies of Biological and Chemical Catalysts* (#TG-MCB090159)  
**Co-PI**; PI: Gregg T. Beckham  
**National Science Foundation XSEDE**; 10/13 – 09/14; Total: 15,452,817 System Units
14. *Inhibition of the Mammalian Glycoprotein YKL-40: Identification of the Physiological Ligand* (#KSEF-148-502-13-307)  
**PI**  
**Kentucky Science and Engineering Foundation**; 07/13 – 06/14; Total: \$30,000
15. *Computational Studies of Biological Systems for Biofuels Applications* (#TG-MCB090159)  
**Co-PI**; PI: Gregg T. Beckham  
**National Science Foundation XSEDE**; 10/12 – 09/13; Total: 14,102,000 System Units
16. *Seed Grant: Insight Into Biomass Conversion from Family 18 Chitinases* (#218425/O10)  
**Co-PI**; PIs: Morten Sørlie and Gregg T. Beckham  
**Research Council of Norway**; 01/12 – 12/12; Total: \$70,000
17. *Understanding Cellulose and Cellulose-Degrading Enzymes and Designing Lignin Deconstruction Catalysts for Biofuels Applications* (#TG-MCB090159)  
**Co-PI**; PI: Gregg T. Beckham  
**National Science Foundation XSEDE**; 10/11 – 09/12; Total: 14,000,000 System Units

## INVITED PRESENTATIONS & PANELS

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1. “Overview of the NSF Division of Chemical, Bioengineering, Environmental, and Transport Systems (CBET),” **NSF Chemistry Division’s Young Investigator Workshop**, Alexandria, VA; May 2023.
2. “Navigating NSF Funding Opportunities and Proposal Writing Tips,” **New York University**, virtual meeting, April 2023.
3. “National Science Foundation Efforts to Address Plastic Pollution and Marine Debris,” **Interagency Marine Debris Coordinating Committee**, virtual meeting, February 2023.
4. “NSF Funding Opportunities and Highlights from the Polymer Circularity Research Portfolio,” **American Chemical Society Fall Meeting**, Chicago, IL; August 2022.
5. “National Science Foundation (NSF): Supporting Science and Engineering Research Towards Solving the “Plastics Problem”,” **U.S. Department of State Interagency Plastic Waste and Scrap Meeting**, virtual meeting; July 2022.
6. “Overview of the NSF Division of Chemical, Bioengineering, Environmental, and Transport Systems (CBET),” **NSF Chemistry Division’s Young Investigator Workshop**, Alexandria, VA; June 2022.
7. “Critical Minerals Research in the NSF Division of Chemical, Bioengineering, Environmental, and Transport Systems,” **Global Expert Mission – Innovate UK**, Washington, DC; May 2022.
8. “World Without Waste: A Circular Bioeconomy,” **NSF Directorate for Biological Sciences Advisory Committee Meeting**, virtual meeting; May 2022.

9. "NSF Funding Opportunities (from the Engineering Perspective)," **University of South Florida Summer Grant Writing Workshop**, virtual workshop, June 2021.
10. "NSF Research Highlights and Funding Opportunities: Solving the 'Plastics Problem'," **American Chemical Society Webinar**, virtual webinar; April 2021.
11. "NSF Funding Opportunities for Biorenewables and Waste Plastic Mitigation Projects," **Emerging Concepts in Biorenewables Panel - hosted by the Center for Biorenewables at The Pennsylvania State University**, virtual panel discussion, December 2020.
12. "Highlights from the NSF Polymeric Materials Synthesis and Degradation Portfolio," **American Institute of Chemical Engineers - Engineering Alternative Technologies Plastic Workshop**, virtual workshop; October 2020.
13. "Highlights from the NSF Polymeric Materials Synthesis and Degradation Portfolio," **Massachusetts Institute of Technology (MIT) Environmental Solutions Initiative Workshop - Plastics and the Environment: Science Meets Public Policy**, virtual workshop, June 2020.
14. "Protein-Carbohydrate Recognition Phenomena Illustrated Through Simulation and Thermodynamic Calculations," **University of Akron**, Chemical and Biomolecular Engineering Department Seminar Series, Akron, OH; February 2020.
15. "Insights into the National Science Foundation's Interfacial Engineering Program and Other Funding Opportunities," **University of Akron**, Chemical and Biomolecular Engineering Department Seminar Series, Akron, OH; February 2020.
16. "Plastics in Engineering Research," **NOAA Interagency Marine Debris Coordinating Committee Biannual Meeting**, virtual meeting; January 2020.
17. "Polymers in Engineering Research," **Triannual Interagency Polymer Working Group Meeting**, Alexandria, VA; January 2020.
18. "Insights into the National Science Foundation's Interfacial Engineering Program and Other Funding Opportunities," **George Washington University**, Civil and Environmental Engineering Department Seminar Series, Washington, DC; November 2019.
19. "Science and Engineering Ethics," **T. C. Williams High School**, Science Department Seminar, Alexandria, VA; May 2019.
20. "Protein-Carbohydrate Recognition Phenomena Illustrated Through Simulation and Thermodynamic Calculations," **University of Connecticut**, Chemical and Biomolecular Engineering Department Seminar Series, Storrs, CT; November 2018.
21. "Insights into the National Science Foundation CAREER Award Mechanism," **University of Kentucky**, Faculty Development Seminar Series, Lexington, KY; April 2018.
22. "The Role of Sex/Gender in Biomedical Engineering Research and Design at the National Science Foundation," **National Science Foundation**, iGIANT roundtable, Alexandria, VA; April 2018.
23. "Biomedical Engineering Funding Opportunities at the National Science Foundation," **Biomedical Engineering Society – 2018 Cellular and Molecular Bioengineering Conference**, Key Largo, FL; January 2018.
24. "Protein-Carbohydrate Recognition Phenomena Illustrated Through Simulation and Thermodynamic Calculations," **University of Kentucky**, Chemistry Department Seminar Series, Lexington, KY; March 2017.
25. "Protein-Carbohydrate Recognition Phenomena Illustrated Through Simulation and Thermodynamic Calculations," **Rutgers University**, Chemical and Biochemical Engineering Department Seminar Series, Piscataway, NJ; February 2017.
26. "Understanding the Protein-Carbohydrate Recognition Mechanisms of Multimodular Enzymes," **The Ohio State University**, Chemical and Biomolecular Engineering Department Seminar Series, Columbus, OH; January 2017.



27. "Understanding the Protein-Carbohydrate Recognition Mechanisms of Multimodular Enzymes," **Clemson University**, Chemical and Biomolecular Engineering Department Seminar Series, Clemson, SC; November 2016.
28. "Understanding the Protein-Carbohydrate Recognition Mechanisms of Multimodular Enzymes," **Northwestern University**, Chemical and Biological Engineering Department Seminar Series, Evanston, IL; November 2016.
29. "Understanding the Protein-Carbohydrate Recognition Mechanisms of Multimodular Enzymes," **University of Kentucky**, Chemical and Materials Engineering Department Seminar Series, Lexington, KY; October 2016.
30. "Understanding the Protein-Carbohydrate Recognition Mechanisms of Multimodular Enzymes," **Vanderbilt University**, Chemical and Biomolecular Engineering Department Seminar Series, Nashville, TN; September 2016.
31. "Understanding Protein-Carbohydrate Recognition Through Molecular Simulation and Enhanced Sampling Free Energy Calculations," **Centre Européen de Calcul Atomique et Moléculaire Workshop – Controlling Food Protein Folding and Aggregation**, Dublin, Ireland, August 2016.
32. "Carbohydrate Recognition Mechanisms of Processive Glycoside Hydrolases," **Tennessee Technological University**, Chemical Engineering Department Seminar Series, Cookeville, TN; February 2016.
33. "The Role of Glycosylated Linkers in Multimodular Cellulase Function," **Cellulosomes, Cellulases, and Other Carbohydrate Modifying Enzymes Gordon Research Conference**, Andover, NH; August 2015.
34. "Glycoside Hydrolase Processivity from a Thermodynamic and Molecular Perspective," **AICHE Annual Meeting, In Honor of Peter T. Cummings Session**, Atlanta, GA; November 2014.
35. "Molecular Mechanisms of Glycoside Hydrolase Polysaccharide Deconstruction," **NSF EPSCoR Membrane Pillar Meeting**, Lexington, KY; October 2014.
36. "Characterizing Glycoside Hydrolase Mechanisms Through Molecular Modeling," **Swedish University of Agricultural Sciences**, Uppsala, Sweden; May 2014.
37. "Characterizing Glycoside Hydrolase Mechanisms Through Molecular Modeling," **Bluegrass Biophysics Symposium**, Lexington, KY; May 2014.
38. "Carbohydrate Recognition Mechanisms of Glycoside Hydrolase Modular Domains," **36<sup>th</sup> Symposium on Biotechnology for Fuels and Chemicals**, Clearwater Beach, FL; May 2014.
39. "Characterizing Glycoside Hydrolase Mechanisms Through Molecular Modeling," **University of Wyoming**, Molecular Biology Department Seminar Series, Laramie, WY; March 2014.
40. "Characterizing Glycoside Hydrolase Mechanisms Through Molecular Modeling," **University of Kentucky**, Molecular and Cellular Biology Department Seminar Series, Lexington, KY; March 2014.
41. "Characterizing Glycoside Hydrolase Mechanisms Through Molecular Modeling," **University of Louisville**, Chemical Engineering Department Seminar Series, Louisville, KY; January 2014.
42. "Mechanisms of Recalcitrant Polysaccharide Deconstruction by Glycoside Hydrolases," **University of Kentucky**, Chemical Engineering Department Seminar Series, Paducah, KY; November 2013.
43. "Molecular Mechanisms of Protein-Protein Abiotic Stress Protection and Plant Cell Wall Deconstruction," **University of Kentucky**, Horticulture Department Seminar Series, Lexington, KY; November 2013.
44. "Characterizing Glycoside Hydrolase Mechanisms Through Molecular Modeling," **4<sup>th</sup> Annual Workshop on Enzymatic Hydrolysis of Insoluble Carbohydrates**, Dragerup, Denmark; September 2013.
45. "Mechanisms of Recalcitrant Polysaccharide Deconstruction by Glycoside Hydrolases," **University of Tennessee**, Center for Renewable Carbon Seminar Series, Knoxville, TN; September 2013.

46. "Computational Investigations of Cellulase and Chitinase Action," **University of York**, Biology Department Seminar Series, York, United Kingdom; November 2012.
47. "Natural Mechanisms for Deconstruction of Recalcitrant Polysaccharides for Biofuels Applications," **University of Portsmouth**, Institute of Biomedical and Biomolecular Science Seminar Series, Portsmouth, United Kingdom; November 2012.
48. "Molecular Mechanisms of Enzymatic Biomass Deconstruction," **University of Kentucky**, Biosystems and Agricultural Engineering Department Seminar Series, Lexington, KY; October 2012.
49. "Insights into Protein/Carbohydrate Interactions from Molecular Simulations," **University of Kentucky**, UK International Society of Pharmaceutical Engineers Chapter Seminar, Lexington, KY; October 2012.
50. "Molecular Simulation for Improved Biomass Deconstruction," **University of Kentucky**, Nanobiotechnology Group Seminar, Lexington, KY; August 2012.

#### CONTRIBUTED PRESENTATIONS

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1. "Determining the Limitations of Processive Polysaccharide Deconstruction by Glycoside Hydrolases," **AIChE Annual Meeting**, Minneapolis, MN; November 2017.
2. "Inhibition and Transglycosylation in *Hypocrea jecorina* Family 3  $\beta$ -glucosidases, Cel3A and Cel3B," **Gordon Research Conference for Cellulases and Other Carbohydrate Modifying Enzymes**, Andover, NH; July 2017.
3. "Carbohydrate Recognition Mechanisms in Cellulose-Specific Type B Carbohydrate Binding Modules," **AIChE Annual Meeting**, San Francisco, CA; November 2016.
4. "The Role of Polar Residues in Processive Chitinase Function," **Swedish Structural Biology Network Annual Conference**, Tällberg, Sweden; June 2016.
5. "The Relationship of Glycoside Hydrolase Ligand Binding Free Energy with Processive Ability," **AIChE Annual Meeting**, Salt Lake City, UT; November 2015.
6. "The Relationship of Glycoside Hydrolase Ligand Binding Free Energy with Processive Ability," **Midwest Enzyme Chemistry Conference**, Chicago, IL; September 2015.
7. "Cello-oligomer Binding Dynamics and Directionality in Family 4 Carbohydrate Binding Modules," **Swedish Structural Biology Network Annual Conference**, Tällberg, Sweden; June 2015.
8. "Ligand Binding Free Energy of Glycoside Hydrolases as a Metric for Processivity and Polysaccharide Morphology Dependence," **Chemical Side of SLU<sup>2+</sup>**, Uppsala, Sweden; August 2014.
9. "Absolute Ligand Binding Free Energy of Glycoside Hydrolases as a Metric for Processivity and Polysaccharide Morphology Dependence," **AIChE Annual Meeting**, San Francisco, CA; November 2013.
10. "Ligand Binding Free Energy of Glycoside Hydrolases as a Metric for Processivity and Polysaccharide Morphology Dependence," **9<sup>th</sup> KY Innovation Entrepreneurship Conference**, Lexington, KY; August 2013.
11. "Ligand Binding Free Energy of Glycoside Hydrolases as a Metric for Processivity and Polysaccharide Morphology Dependence," **Gordon Research Conference for Cellulases, Cellulosomes, and Other Carbohydrate Modifying Enzymes**, Andover, NH; August 2013.
12. "Absolute Ligand Binding Free Energy of Glycoside Hydrolases as a Metric for Processivity and Polysaccharide Morphology Dependence," **35<sup>th</sup> Symposium on Biotechnology for Fuels and Chemicals**, Portland, OR; May 2013.
13. "Absolute Ligand Binding Free Energy of Glycoside Hydrolases as a Metric for Processivity and Polysaccharide Morphology Dependence," **NSF Bioinformatics Workshop**, Little Rock, AR; March 2013.

14. "Identification of Molecular-Level Contributions to Processivity in Glycoside Hydrolases From Computational and Experimental Studies of *Serratia Marcescens* Chitinases," **AICHE Annual Meeting**, Pittsburgh, PA; October 2012.
15. "Insights into the Molecular-Level Mechanism of a Processive, Glycosylated Cellulase from Molecular Simulation," **34<sup>th</sup> Symposium on Biotechnology for Fuels and Chemicals**, New Orleans, LA; April 2012.
16. "Insights into the Molecular-Level Mechanism of a Processive, Glycosylated Cellulase from Molecular Simulation," **ACS Spring Meeting**, San Diego, CA; March 2012.
17. "Decrystallization Thermodynamics of Four Common Cellulose Polymorphs and  $\alpha$ -Chitin," **AICHE Annual Meeting**, Minneapolis, MN; October 2011.
18. "The Role of Aromatic Residues in the Catalytic Domain Tunnel of *Hypocrea jecorina* Cellobiohydrolase Cel6A," **AICHE Annual Meeting**, Minneapolis, MN; October 2011.
19. "Characterization of Thermal Stability In Endoglucanases with Bioinformatics, Molecular Simulation, and Rosetta Design," **AICHE Annual Meeting**, Minneapolis, MN; October 2011.
20. "Molecular Simulations for Improved Biomass Conversion," Chemical and Materials Engineering Fall 2011 Seminar Series, **University of Kentucky**, Lexington, KY; August 2011.
21. "Nanoscale Decrystallization Thermodynamics of Four Common Cellulose Polymorphs and  $\alpha$ -Chitin," **ACS Fall Meeting**, Denver, CO; August 2011.
22. "The Role of Aromatic Residues in the Catalytic Domain Tunnel of *Hypocrea jecorina* Cellobiohydrolase Cel6A," **Gordon Research Conference for Cellulases, Cellulosomes, and Other Carbohydrate Modifying Enzymes**, Easton, MA; July 2011.
23. "Fluidized Bed Steam Reforming Technology Demonstration for Conversion of Savannah River Tank 48 Waste to a Granular Carbonate Product," **Waste Management Symposia**, Phoenix, AZ; March 2010.
24. "Fluidized Bed Steam Reforming Technology Demonstration for Conversion of Savannah River Tank 48 Waste to a Granular Carbonate Product," **URS**, Denver, CO; February 2010.
25. "The National Energy Technology Contract Win," **URS**, Denver, CO; October 2009.
26. "Molecular Dynamics Simulation of a Nanoscale Device for Fast Sequencing of DNA," **Fall Creek Falls Conference**, Nashville, TN; September 2007.
27. "Molecular Dynamics Simulation of a Nanoscale Device for Fast Sequencing of DNA," **Eleventh International Conference on Properties and Phase Equilibria for Product and Process Design (PPEPPD)**, Crete, Greece; May 2007.
28. "Molecular Dynamics Simulation of a Nanoscale Device for Fast Sequencing of DNA," **AICHE Annual Meeting**, San Francisco, CA; November 2006.
29. "Molecular Dynamics Simulation of a Nanoscale Device for Fast Sequencing of DNA," **VINSE Nanoday**, Nashville, TN; November 2006.
30. "Molecular Dynamics Simulation of a Nanoscale Device for Fast Sequencing of DNA," **Foundations of Molecular Modeling and Simulation (FOMMS) 2006**, Blaine, WA; July 2006.
31. "Molecular Dynamics Simulation of a Nanoscale Device for Fast Sequencing of DNA," **DOE CSGF Annual Meeting**, Washington, DC; June 2006.
32. "Molecular Dynamics Simulation of a Nanoscale Device for Fast Sequencing of DNA," **AICHE Annual Meeting**, Cincinnati, OH; November 2005.
33. "Molecular Dynamics Simulation of a Nanoscale Device for Fast Sequencing of DNA," **VINSE Nanoday**, Nashville, TN; November 2005.
34. "Molecular Dynamics Simulation of a Nanoscale Device for Fast Sequencing of DNA," **DOE CSGF Annual Meeting**, Washington, DC; June 2005.
35. "Car-Parrinello Molecular Dynamics Simulation of Metal Oxide/Water Interfaces," **VINSE Nanoday**, Nashville, TN; November 2004.

36. "Car-Parrinello Molecular Dynamics Simulation of Metal Oxide/Water Interfaces," **DOE CSGF Annual Meeting**, Washington, DC; June 2004.
37. "Evaluating the Consistency of Thermodynamic Data for Aqueous-HF at 1 atm Via Molecular Simulation and a Thermodynamic Model," **FOMMS 2003**, Keystone, CO; July 2003.
38. "Evaluating the Thermodynamic Consistency of Aqueous Hydrogen Fluoride Data at 101.325 kPa," **AICHe Annual Meeting**, Indianapolis, IN; November 2002.
39. "Evaluating the Thermodynamic Consistency of an Aqueous-HF System Using the SAFT-VR Model," **AICHe Student Regional Meeting**, Blacksburg, VA; April 2002.

## CONTRIBUTED STUDENT PRESENTATIONS & POSTERS

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*Student presenter is underlined*

1. J. Gado, G. T. Beckham, C. M. Payne, "Exploring Glycoside Hydrolase Family 7 Cellulases with Machine Learning," invited presentation at the **Society of Industrial Microbiology's 44<sup>th</sup> Symposium on Biomaterials, Fuels and Chemicals**, New Orleans, LA, May 2022.
2. J. Gado, B. E. Harrison, M. Sandgren, J. Ståhlberg, G. T. Beckham, and C. M. Payne, "Understanding Sequence and Structure Diversity in family 7 Glycoside Hydrolases with Machine Learning," invited presentation at the **Gordon Research Conference on Carbohydrate Active Enzymes for Glycan Conversions**, Andover, NH; July 2021.
3. J. Gado, G. T. Beckham, and C. M. Payne, "Turn up the Heat: PETases for High Temperature Applications," **2<sup>nd</sup> Biennial Symposium on Microbial Carbon Valorization**, Golden, CO; 2019.
4. J. Gado, G. T. Beckham, and C. M. Payne, "Machine Learning Predicts Functional Classes of Family 7 Glycoside Hydrolases with High Accuracy," **Lignin Symposium**, Golden, CO; May 2019.
5. L. Mills, G. T. Beckham, and C. M. Payne, "The Hydrophobicity and Conformations of Common Glycosylation Motifs across the Kingdoms of Life," **AICHe Annual Meeting**, Pittsburgh, PA; October 2018.
6. J. Gado, A. Borisova, J. Stahlberg, and C. M. Payne, "Machine Learning Predicts Functional Classes of Family 7 Glycoside Hydrolases with High Accuracy," **AICHe Annual Meeting**, Pittsburgh, PA; October 2018.
7. L. Mills, G. T. Beckham, and C. M. Payne, "The Hydrophobicity and Conformations of Common Glycosylation Motifs across the Kingdoms of Life," **Materials and Chemical Engineering (MACE) Graduate Student Symposium**, Lexington, KY; April 2018.
8. L. Mills, G. T. Beckham, and C. M. Payne, "The Hydrophobicity and Conformations of Common Glycosylation Motifs across the Kingdoms of Life," **44<sup>th</sup> Annual NAFF Symposium**, Lexington, KY; March 2018.
9. Y. Yu and C. M. Payne, "Conformational Changes of 2'-hydroxybiphenyl-2-sulfinate Desulfinate," **AICHe Annual Meeting**, Minneapolis, MN; November 2017.
10. L. Mills, C. M. Payne, and D. Englert, "Understanding the Role of Conformational Change in Product Inhibition of 2-(2'-hydroxybiphenyl)Benzenesulfinate Desulfinate (DszB)," **AICHe Annual Meeting**, Minneapolis, MN; November 2017.
11. A. A. Kognole and C. M. Payne, "Cellulose-specific Type B Carbohydrate Binding Modules: Understanding Substrate Recognition Mechanisms Through Molecular Simulation," **Gordon Research Conference for Cellulases and Other Carbohydrate Modifying Enzymes**, Andover, NH; July 2017.
12. A. A. Kognole and C. M. Payne, "Understanding Substrate Recognition Mechanisms in Type B Carbohydrate Binding Modules Through Molecular Simulation," **6<sup>th</sup> Annual Bluegrass Molecular Biophysics Symposium**, Lexington, KY; May 2017.

13. Y. Yu and C. M. Payne, "Conformational Changes of 2'-hydroxybiphenyl-2-sulfinate Desulfinate," **6<sup>th</sup> Annual Bluegrass Molecular Biophysics Symposium**, Lexington, KY; May 2017.
14. A. A. Kognole and C. M. Payne, "Understanding Substrate Recognition Mechanisms in Type B Carbohydrate Binding Modules Through Molecular Simulation," **Materials and Chemical Engineering Graduate Student Symposium**, Lexington, KY; May 2017. << A. A. Kognole recipient of outstanding graduate student research award >>.
15. L. C. Mills, D. L. Englert, and C. M. Payne, "Conformational Change of 2-(2'-hydroxyphenyl)benzenesulfinate Desulfinate During Catalysis," **8<sup>th</sup> Annual Southeast Enzyme Conference**, Atlanta, GA; April 2017.
16. Y. Yu and C. M. Payne, "Conformational Changes of 2'-hydroxybiphenyl-2-sulfinate Desulfinate," **8<sup>th</sup> Annual Southeast Enzyme Conference**, Atlanta, GA; April 2017.
17. I. Isaksen, S. Jana, C. M. Payne, and Å. Røhr, "Computational Study of the Protonation States of the Conserved His172 in the Lytic Polysaccharide Monooxygenase ScLPMO10B," **53<sup>rd</sup> NBS Contact Meeting**, Storefjell (Gol), Norway; January 2017.
18. Y. Yu and C. M. Payne, "The Relationship of Conformational Changes in 2'-hydroxybiphenyl-2-sulfinate (HBPS) Desulfinate (DszB) to Product Inhibition," **Tracy Farmer Institute for Sustainability and the Environment 6<sup>th</sup> Annual Sustainability Forum**, Lexington, KY; December 2016.
19. Y. Yu and C. M. Payne, "Molecular Dynamics Simulations Revealed Conformational Changes in 2'-hydroxybiphenyl-2-sulfinate (HBPS) Desulfinate (DszB) Related to Product Inhibition," **Ashland Inc. Distinguished Lectures and Drug Discovery and Development Symposium**, Lexington, KY; November 2016.
20. A. A. Kognole and C. M. Payne, "Inhibition of the Mammalian Glycoprotein YKL-40: Identification of the Physiological Ligand," **Ashland Inc. Distinguished Lectures and Drug Discovery and Development Symposium**, Lexington, KY; November 2016.
21. S. Jana, A. G. Hamre, M. Sørli, and C. M. Payne, "The Relationship Between Chitinase Binding Affinity, Processivity, and Work Required to Decrystallize  $\beta$ -chitin," **AIChE Annual Meeting**, San Francisco, CA; November 2016.
22. N. T. Anderson, A. Nutt, M. H. Momeni, P. Våljamäe, G. Johansson, J. Ståhlberg, and C. M. Payne, "o-Nitrophenyl Cellobioside as an Active Site Probe for Family 7 Cellobiohydrolases," **AIChE Annual Meeting**, San Francisco, CA; November 2016.
23. Y. Yu and C. M. Payne, "The Relationship of Conformational Changes in 2'-hydroxybiphenyl-2-sulfinate (HBPS) Desulfinate (DszB) to Product Inhibition," **Midwest Enzyme Chemistry Conference**, Chicago, IL; October 2016.
24. S. Jana, A. G. Hamre, M. Sørli, and C. M. Payne, "The Relationship Between Chitinase Binding Affinity, Processivity, and Work Required to Decrystallize  $\beta$ -chitin," **Midwest Enzyme Chemistry Conference**, Chicago, IL; October 2016.
25. A. A. Kognole and C. M. Payne, "Cellulose-specific Type B Carbohydrate Binding Modules: Understanding Substrate Recognition Mechanisms Through Molecular Simulation," **Midwest Enzyme Chemistry Conference**, Chicago, IL; October 2016.
26. I. Isaksen, S. Jana, C. M. Payne, and Å. Røhr, "Protonation States of Conserved Amino Acids in the Lytic Polysaccharide Monooxygenase ScLPMO10B," **Annual BioStruct Conference**, Inderøy, Norway; August 2016.
27. A. A. Kognole and C. M. Payne, "Cellulose-specific Type B Carbohydrate Binding Modules: Understanding Substrate Recognition Mechanisms Through Molecular Simulation," **Gordon Research Conference for Computational Chemistry**, Girona, Spain; July 2016.
28. A. A. Kognole and C. M. Payne, "Inhibition of the Mammalian Glycoprotein YKL-40: Identification of the Physiological Ligand," **Gordon Research Conference for Computational Chemistry**, Girona, Spain; July 2016.

29. Y. Yu, I. Fursule, L. C. Mills, D. L. Englert, B. J. Berron, and C. M. Payne, "Force Field Parameterization of 2'-hydroxybiphenyl-2-sulfinate, 2-hydroxybiphenyl, and Related Analogs," **Swedish Structural Biology Network Annual Conference**, Tällberg, Sweden; June 2016.
30. L. C. Mills, D. L. Englert, and C. M. Payne, "Conformational Change of 2-(2'-hydroxyphenyl)benzenesulfinate Desulfinate During Catalysis," **Swedish Structural Biology Network Annual Conference**, Tällberg, Sweden; June 2016.
31. N. T. Anderson, A. Nutt, M. H. Momeni, P. Våljamäe, G. Johansson, J. Ståhlberg, and C. M. Payne, "o-Nitrophenyl Cellobioside as an Active Site Probe for Family 7 Cellobiohydrolases," **Swedish Structural Biology Network Annual Conference**, Tällberg, Sweden; June 2016.
32. S. Jana and C. M. Payne, "The Relationship Between Chitinase Binding Affinity, Processivity, and Work Required to Decrystallize  $\beta$ -chitin," **Materials and Chemical Engineering Graduate Student Symposium**, Lexington, KY; May 2016. << *S. Jana recipient of graduate student research award* >>
33. S. Jana and C. M. Payne, "The Relationship Between Chitinase Binding Affinity, Processivity, and Work Required to Decrystallize  $\beta$ -chitin," **Naff Symposium**, Lexington, KY; April 2016.
34. A. A. Kognole and C. M. Payne, "Inhibition of the Mammalian Glycoprotein YKL-40: Identification of the Physiological Ligand," **Center for Clinical and Translational Science Spring Symposium**, Lexington, KY; April 2016.
35. Y. Yu and C. M. Payne, "CHARMM Additive All-Atom Force Field for 2-(2'-hydroxyphenyl) benzenesulfinate, 2-hydroxybiphenyl, and Related Analogs," **Materials and Chemical Engineering Graduate Student Fall Symposium**, Lexington, KY; September 2015.
36. I. Geronimo, C. Denning, D. Heidary, E. C. Glazer, and C. M. Payne, "Molecular Determinants of Substrate Specificity in Cytochrome P450<sub>BM3</sub>," **Midwest Enzyme Chemistry Conference**, Chicago, IL; September 2015.
37. A. A. Kognole and C. M. Payne, "Cello-oligomer Binding Dynamics and Directionality in Family 4 Carbohydrate Binding Modules," **Gordon Research Conference for Cellulases, Cellulosomes, and Other Carbohydrate Modifying Enzymes**, Andover, NH; August 2015.
38. S. Jana, A. G. Hamre, M. M. Holen, G. Mathiesen, M. Sørli, and C. M. Payne, "The Relationship of Glycoside Hydrolase Ligand Binding Free Energy to Processive Ability," **Gordon Research Conference for Cellulases, Cellulosomes, and Other Carbohydrate Modifying Enzymes**, Andover, NH; August 2015.
39. I. Geronimo, C. Denning, D. Heidary, E. C. Glazer, and C. M. Payne, "Identification of Stabilizing Interactions and Labile Regions in Cytochrome P450<sub>BM3</sub>," **Foundations of Molecular Modeling and Simulation**, Mount Hood, Oregon; July 2015.
40. I. Geronimo, C. Denning, D. Heidary, E. C. Glazer, and C. M. Payne, "Identification of Stabilizing Interactions and Labile Regions in Cytochrome P450<sub>BM3</sub>," **Swedish Structural Biology Network Annual Conference**, Tällberg, Sweden; June 2015.
41. A. A. Kognole and C. M. Payne, "Inhibition of the Mammalian Glycoprotein YKL-40: Identification of the Physiological Ligand," **Swedish Structural Biology Network Annual Conference**, Tällberg, Sweden; June 2015.
42. S. Jana, A. G. Hamre, N. K. Reppert, M. Sørli, and C. M. Payne, "The Role of Polar Residues in Substrate Positioning, Binding, and Processivity in a Family 18 *Serratia marcescens* Chitinase," **Swedish Structural Biology Network Annual Conference**, Tällberg, Sweden; June 2015.
43. I. Geronimo, C. Denning, D. Heidary, E. C. Glazer, and C. M. Payne, "Identification of Stabilizing Interactions and Labile Regions in Cytochrome P450<sub>BM3</sub>," **Kentucky EPSCoR Annual Conference**, Lexington, KY; May 2015.
44. A. A. Kognole and C. M. Payne, "Inhibition of the Mammalian Glycoprotein YKL-40: Identification of the Physiological Ligand," **Materials and Chemical Engineering Graduate Student Spring Symposium**, Lexington, KY; May 2015.

45. S. Jana, A. G. Hamre, N. K. Reppert, M. Sørлие, and C. M. Payne, "The Role of Polar Residues in Substrate Positioning, Binding, and Processivity in a Family 18 *Serratia marcescens* Chitinase," **Materials and Chemical Engineering Graduate Student Spring Symposium**, Lexington, KY; May 2015.
46. A. A. Kognole and C. M. Payne, "Inhibition of the Mammalian Glycoprotein YKL-40: Identification of the Physiological Ligand," **Bluegrass Biophysics Symposium**, Lexington, KY; May 2015.
47. S. Jana, A. G. Hamre, M. M. Holen, G. Mathiesen, M. Sørлие, and C. M. Payne, "The Relationship of Glycoside Hydrolase Ligand Binding Free Energy to Processive Ability," **Bluegrass Biophysics Symposium**, Lexington, KY; May 2015.
48. T. O. Karnes and C. M. Payne, "Substrate Specificity and Inhibition in Enzymatic Desulfurization of Petroleum," **AIChE Southern Student Regional Conference**, Clearwater Beach, FL; April 2015.
49. S. Jana, A. G. Hamre, P. Wildberger, M. M. Holen, G. T. Beckham, M. Sørлие, and C. M. Payne, "The Role of Carbohydrate-Aromatic Interactions in *Serratia marcescens* Chitinases," **AIChE Annual Meeting**, Atlanta, GA; November 2014.
50. A. A. Kognole and C. M. Payne, "Ligand Binding Dynamics and Directionality in *Cellulomonas fimi* Family 4 Carbohydrate Binding Modules," **AIChE Annual Meeting**, Atlanta, GA; November 2014.
51. A. A. Kognole and C. M. Payne, "Inhibition of the Mammalian Glycoprotein YKL-40: Identification of the Physiological Ligand," **AIChE Annual Meeting**, Atlanta, GA; November 2014.
52. A. A. Kognole and C. M. Payne, "Ligand Binding Dynamics and Directionality in *Cellulomonas fimi* Family 4 Carbohydrate Binding Modules," **Materials and Chemical Engineering Graduate Student Fall Symposium**, Lexington, KY; September 2014.
53. S. Jana, A. G. Hamre, P. Wildberger, M. M. Holen, G. T. Beckham, M. Sørлие, and C. M. Payne, "The Role of Carbohydrate-Aromatic Interactions in *Serratia marcescens* Chitinases," **Natural Products Consortium Symposium**, Lexington, KY; August 2014.
54. A. A. Kognole and C. M. Payne, "Ligand Binding Dynamics and Directionality in *Cellulomonas fimi* Family 4 Carbohydrate Binding Modules," **Bluegrass Biophysics Symposium**, Lexington, KY; May 2014.
55. S. Jana, A. G. Hamre, P. Wildberger, M. M. Holen, G. T. Beckham, M. Sørлие, and C. M. Payne, "The Role of Carbohydrate-Aromatic Interactions in *Serratia marcescens* Chitinases," **Bluegrass Biophysics Symposium**, Lexington, KY; May 2014.

## TEACHING EXPERIENCE

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Spring 2017	Product and Process Design II (CME 456 – 4 credit hours)
Fall 2016	Professionalism, Ethics, and Safety (CME 470 – 2 credit hours)
Fall 2016	Chemical Engineering Laboratory II (CME 433 – 3 credit hours, team-taught)
Fall 2016	Special Problems in Chemical Engineering (CME 395 – 1 credit hour)
Spring 2016	Engineering Thermodynamics (CME 320 – 4 credit hours)
Spring 2016	Chemical Engineering Laboratory I (CME 432 – 2 credit hours, team-taught)
Fall 2015	Professionalism, Ethics, and Safety (CME 470 – 2 credit hours)
Fall 2015	Special Problems in Chemical Engineering (CME 395 – 3 credit hours)
Fall 2015	Chemical Engineering Seminar (CME 771 – 0 credit hour)
Spring 2015	Engineering Thermodynamics (CME 320 – 4 credit hours)
Spring 2015	Special Problems in Chemical Engineering (CME 395 – 3 credit hours)
Spring 2015	Chemical Engineering Laboratory I (CME 432 – 2 credit hours, team taught)
Fall 2014	Professionalism, Ethics, and Safety (CME 470 – 2 credit hours)
Fall 2014	Special Problems in Chemical Engineering (CME 395 – 1 credit hour)

*Christina Payne, PE, PhD*

Spring 2014	Engineering Thermodynamics (CME 320 – 4 credit hours)
Spring 2014	Special Problems in Chemical Engineering (CME 395 – 3 credit hours)
Spring 2014	Chemical Engineering Laboratory I (CME 432 – 2 credit hours, team taught)
Fall 2013	Professionalism, Ethics, and Safety (CME 470 – 2 credit hours)
Spring 2013	Engineering Thermodynamics (CME 320 – 4 credit hours)
2008 - 2009	Girls Exploring Science, Technology, Engineering, and Mathematics
2005 - 2007	Pencil Foundation, Math and reading tutoring
2002 - 2003	Vanderbilt University Teaching Assistant, Chemical Engineering Unit Operations

## STUDENTS MENTORED

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### *Postdoctoral*

Inacrist Geronimo, PhD, Chemistry, Lodz University of Technology, Poland; 2014 - 2018

### *Graduate*

Japheth Gado, PhD, Chemical Engineering, 2016 – 2020 (defended November 2020)

Suvamay Jana, PhD, Chemical Engineering, 2012 – 2016 (defended December 14, 2016)

Abhishek Kognole, PhD, Chemical Engineering, 2012 – 2017 (defended September 25, 2017)

Landon Mills, seeking PhD, Chemical Engineering, 2014 – present (defended July 10, 2019)

Yue Yu, PhD, Chemical Engineering, 2014 – 2017 (defended December 6, 2017)

### *Visiting PhD Students*

Ingvild Isaksen, Chemistry, Biotechnology, and Food Science – Norwegian University of Life Sciences

- January 2016 – July 2016

István Tamás, Department of Medical Chemistry – University of Debrecen, Hungary

- April 2017 – August 2017

### *Undergraduate Researchers*

Nolan Anderson, BS, Chemical Engineering, 2013 – 2017

- Publication in *FEBS Lett.* (<https://dx.doi.org/10.1002/1873-3468.12027>)
- Graduate student at Univ. California - Santa Barbara, 2017 – present

Robert Brooks, BS, Chemical Engineering, 2015

Codell Gibson, BS, Chemical Engineering, 2013 – 2014

Dylan Gilley, BS, Chemical Engineering, 2016 – 2017

- Graduate student at Purdue University, 2020 – present

Tyler Karnes, BS, Chemical Engineering, 2014 – 2015

- 2014 John Walker Biology and Engineering Award for Undergraduate Research (\$1,000)

Shawn Nigam, BS, Chemistry, 2015 – 2016

- Publication in *Chem. Sci.* (<https://doi.org/10.1039/C7SC00496F>)

Demarcus Smiley, BS, Chemical Engineering, 2016 – 2017

Devin Wren, BS, Chemical Engineering, 2015 – 2017



## PROFESSIONAL AND COMMUNITY SERVICE

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### **Professional Society Offices Held**

- AIChE – Computational Molecular Science and Engineering Forum; Liaison Director (2016 – 2018)

### **Conference Organization**

- Co-Chair, “Federally-Funded Research for Polymer Circularity,” American Chemical Society Fall Meeting, Chicago, IL, 2022.
- Chair, “Strategies for Micro- and Nano-plastics Mitigation, Remediation, and Recycling,” Asia-Pacific Economic Cooperation (APEC) Workshop on Nanoplastics in Marine Debris in the APEC Region, virtual workshop, 2021.
- Steering Committee Member, “Responding to Plastic Pollution through Science: From Research to Action,” Inaugural Workshop of the French-American Research Partnership on Nano-, Micro-, and Macro-Plastic Pollution, Le Mans, France, 2019
- Co-Chair, “Poster Session: Computational Molecular Science and Engineering Forum (CoMSEF),” AIChE Annual Meeting, Minneapolis, MN, 2017
- Chair, “Thermophysical Properties of Biological Systems,” AIChE Annual Meeting, San Francisco, CA, 2016
- Co-Chair, “Thermophysical Properties and Phase Behavior III,” AIChE Annual Meeting, San Francisco, CA, 2016
- Chair, “Thermophysical Properties of Biological Systems,” AIChE Annual Meeting, Salt Lake City, UT, 2015
- Co-Chair, “Thermophysical Properties and Phase Behavior III,” AIChE Annual Meeting, Salt Lake City, UT, 2015
- Chair, “Thermophysical Properties of Biological Systems,” AIChE Annual Meeting, Atlanta, GA, 2014
- Chair, “Thermophysical Properties of Biological Systems,” AIChE Annual Meeting, San Francisco, CA, 2013
- Co-Chair, “Multiscale and Molecular Modeling for Renewable Energy Systems,” AIChE Annual Meeting, San Francisco, CA, 2013
- Co-Chair, “Enzyme Science and Technology,” 35<sup>th</sup> Symposium on Biotechnology for Fuels and Chemicals, Portland, OR, 2013
- Chair, “Thermodynamics of Energy Systems,” AIChE Annual Meeting, Pittsburgh, PA, 2012.
- Co-Chair, “Thermodynamics of Energy Systems,” AIChE Annual Meeting, Minneapolis, MN, 2011.

### **University of Kentucky Service**

Member, University Infrastructure Task Force Strategic Planning Committee, 2017

Member, Department of Chemical Engineering Strategic Planning Committee, 2016 – 2017

College of Engineering Senator, University Senate, 2015 – 2017

Member, University Senate Research and Graduate Education Committee, 2015 – 2017

Member, Center for Computational Sciences Planning and Allocations Committee, 2013 – 2017

Member, Department of Chemical Engineering Graduate Studies Committee, 2012 – 2017

College of Engineering Associate Dean for Research and Graduate Studies Selection Committee, 2015

### **PhD Advisory Committee Service**

External member, Kirtley Amos, Horticulture, 2016 – 2017  
Departmental member, Andrew Placido, Chemical Engineering, 2014 – 2017  
Departmental member, Leila Safazadeh, Chemical Engineering, 2014 – 2016  
External examiner, William Serson, Plant Physiology, 2017  
External member, Bradley Stewart, Chemistry, 2015 – 2017  
External examiner, Jiwen Zhang, Civil Engineering, 2016

### **Peer Reviewer for Funding Agencies**

American Chemical Society Petroleum Research Fund  
Department of Energy - Advanced Manufacturing Office  
Department of Energy - Bioenergy Technologies Office  
Department of Energy Computational Science Graduate Fellowship Program  
Kentucky NSF EPSCoR  
National Science Foundation  
National Science Foundation XSEDE Resource Allocation Committee, 2012 – 2017  
Natural Sciences and Engineering Research Council of Canada (NSERC)  
University of Leuven, Belgium Industrial Research Council

### **Peer Reviewer for Journals**

3 Biotech; ACS Sustainable Chemistry & Engineering; AIMS Materials Science; Biochimica et Biophysica Acta – Proteins and Proteomics; Biochemistry; Biochemical Engineering Journal; Biomacromolecules; Biotechnology and Bioengineering; Biotechnology for Biofuels; Biophysical Journal; Computational Biology and Chemistry; Current Opinion in Chemical Biology; Energy & Fuels; FEBS Journal; International Journal of Molecular Sciences; International Journal of Bioinformatics Research and Applications; Journal of the American Chemical Society; Journal of Biological Chemistry; Journal of Molecular Graphics and Modelling; Journal of Physical Chemistry B; Journal of Scientific Review; Journal of Structural Biology; Molecular Biotechnology; Molecular Simulation; Nature Chemistry; Science; Science Advances; Scientific Reports

### **Consulting**

Spherix Consulting: Reviewed feasibility of a drug delivery process design (2014)

### **Community Outreach and Broadening Participation Activities**

- Alexandria City Public Schools Science Fair Mentor – Alexandria, VA – September 2018 –present
- Alexandria City Public Schools Science and Engineering Ethics Workshop – Alexandria City High School, Alexandria, VA – May 2023
- Alexandria City Public Schools Science Fair Judge – Alexandria City High School, Alexandria, VA – January 2023
- Science Buddies “Ask an Expert” online science fair forum advisor – <https://www.sciencebuddies.org> August 2020 – 2023
- Alexandria City Public Schools Science Fair Judge – Alexandria City High School, Alexandria, VA – January 2022
- Alexandria City Public Schools Science Fair Judge – T. C. Williams High School, Alexandria, VA – January 2021

*Christina Payne, PE, PhD*

- Alexandria City Public Schools Science and Engineering Ethics Workshop – T. C. Williams High School, Alexandria, VA – June 2020
- Alexandria City Public Schools STEM-H Careers Virtual Seminar Series – T. C. Williams High School, Alexandria, VA – April 2020
- Alexandria City Public Schools Science Fair Judge – T. C. Williams High School, Alexandria, VA – January 2020
- Alexandria City Public Schools Science and Engineering Ethics Workshop – T. C. Williams High School, Alexandria, VA – May 2019
- Alexandria City Public Schools Science Fair Judge – T. C. Williams High School, Alexandria, VA – January 2019
- USA Science and Engineering Festival, Meet the Scientists Session – Washington, DC – April 2018
- Alexandria City Public Schools Science Fair Judge – T. C. Williams High School, Alexandria, VA – January 2018
- Organization of Expanding Your Horizons “STEM Opportunity Fair” for middle school girls – Univ. Kentucky – April 2017
- Molecular Modeling demonstration for K-12 students – Univ. of Kentucky Engineering Day event – Feb. 2017
- Girls in Engineering, Math, and Science (Girl Scout/University of Kentucky STEM event); “Biology’s scissors: Turning sugars into energy with enzymes” – Nov. 2016
- Molecular Modeling demonstration for K-12 students – Univ. of Kentucky Engineering Day event – Feb. 2016
- Girls in Engineering, Math, and Science (Girl Scout/University of Kentucky STEM event); “Biology’s scissors: Turning sugars into energy with enzymes” – Nov. 2015
- Molecular Modeling demonstration for K-12 students (with undergraduate researcher Nolan Anderson) – Univ. of Kentucky Engineering Day event – Feb. 2015
- Girls in Engineering, Math, and Science (Girl Scout/University of Kentucky STEM event); “Biology’s scissors: Turning sugars into energy with enzymes” – Nov. 2014
- Society of Women Engineers (SWE) Quiz Bowl Moderator – University of Kentucky – April 2014
- Molecular Modeling demonstration for K-12 students – Univ. of Kentucky Engineering Day event – Feb. 2014
- Girls in Engineering, Math, and Science (Girl Scout/University of Kentucky STEM event); “Super Shape-Memory Materials” – Nov. 2013