Jim Pfaendtner

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I. PROFESSIONAL PREPARATION

NSF International Postdoctoral Fellowship Program, 2007—2009
Project focus: *Multiscale modeling of conformational change in macromolecular assemblies*
Advisors: Prof. Dr. Michele Parrinello (ETH Zürich) and Prof. Gregory A. Voth (University of Utah)

Ph.D. Chemical Engineering, 2007
Dissertation: *Mechanistic Modeling of Hydrocarbon Autoxidation: Theory and Application to the Study of Lubricant Degradation*
Advisor: Dr. Linda J. Broadbelt (Northwestern University)

B.S. Chemical Engineering, with highest honors, 2001
Georgia Institute of Technology, Atlanta, GA

II. APPOINTMENTS

2020–present Professor of Chemistry, University of Washington
2019–present Department Chair, Chemical Engineering, University of Washington
Professor of Chemical Engineering, University of Washington
Steven R. and Connie R. Rogel Endowed Professor of Chemical Engineering
2018–present Associate Vice Provost for Research Computing, University of Washington
2015–2019 Associate Professor of Chemical Engineering, University of Washington
2016–2019 Jagjeet and Janice Bindra Endowed Career Development Professor
2014–2016 Steven R. and Connie R. Rogel Endowed Faculty Fellow
2017–present Senior Data Science Fellow, eScience Institute, University of Washington
2016–present Senior Scientist, Pacific Northwest National Laboratory
2013–2020 Adjunct Professor of Chemistry, University of Washington
2009–2015 Assistant Professor of Chemical Engineering, University of Washington
2001–2003 Process engineer and industrial hygiene consultant, 3M Company

III. HONORS AND AWARDS

2014 UW College of Engineering Faculty Junior Innovator Award
2014 NSFC Research Fellowship for International Young Scientists
2013 NAE Frontiers of Engineering Education Participant
2013 University of Washington Presidential Distinguished Teaching Award
2013 ACS COMP OpenEye Outstanding Junior Faculty Award
2012 National Science Foundation CAREER Award
2012 National Academy of Sciences Kavli Fellow
2011 ACS PRF Doctoral New Investigator Award

2007 NSF International Research Fellowship

IV. PUBLICATIONS *(superscript denotes graduate students[1], postdocs[2], undergraduates[3] from my group)*

Refereed archival journal publications

95. S. Summers, C. Kraft, S. Alamdari[1], J. Pfaendtner, J. Kaar, "Enhanced Activity and Stability of Acidothermus cellulolyticus Endoglucanase 1 in Ionic Liquids via Engineering Active Site Residues and Non-native Disulfide Bridges", *ACS Sus. Chem & Eng*, **2020,** *in press.*
94. E.L. Buckle, J. Sampath[2], N. Michael, S.D. Whedon, C.J.A. Leonen, J. Pfaendtner, G. Drobny, C. Chatterjee, "Trimethylation of the R5 silica-precipitating peptide increases silica particle size by redirecting orthosilicate binding," *ChemBioChem*, **2020**, *in press*.
93. J. Smith[1], J. Pfaendtner, "Elucidating the molecular interactions between uremic toxins and the Sudlow II binding site of human serum albumin," *J. Phys. Chem. B*, **2020,** 124(19), 3922-3930. DOI: 10.1021/acs.jpcb.0c02015
92. J. Sampath[2], A. Kullman[1], R. Gebhart, G. Drobny, J. Pfaendtner, "Molecular recognition and specificity of biomolecules to titanium dioxide from molecular dynamics simulations," *npj Comput. Mater.* **2020**, 6(34), DOI: 10.1038/s41524-020-0288-7
91. B. Hellner, S. Alamdari[1], H. Pyles, S. Zhang, A. Prakash[1], K. G. Sprenger[1], J. DeYoreo, D. Baker, J. Pfaendtner, F. Baneyx, "Sequence–Structure–Binding Relationships Reveal Adhesion Behavior of the Car9 Solid-Binding Peptide: An Integrated Experimental and Simulation Study," *J. Am. Chem. Soc.* **2020**, 142(5), 2355-2363. DOI: 10.1021/jacs.9b11617
90. S. Alamdari[1], J. Pfaendtner, "Impact of glutamate carboxylation in the adsorption of the α-1 domain of osteocalcin to hydroxyapatite and titania," *Mol. Syst. Des. Eng.* **2020**, 5, 620-631. DOI: 10.1039/C9ME00158A
89. J. Smith[1], P. McMullen, Z. Yuan, J. Pfaendtner, S. Jiang, "Elucidating Molecular Design Principles for Charge-Alternating Peptides," *Biomacromolecules* **2020**, 21(2), 435-443. DOI: 10.1021/acs.biomac.9b01191
88. J. Sampath[2], J. Pfaendtner, "Amphiphilic peptide binding on crystalline vs. amorphous silica from molecular dynamics simulations," *Mol. Phys.* **2019**, 117(23-24), 3642-3650. DOI: 10.1080/00268976.2019.1657192
87. P. Emani, Y. Yimer[2], S. Davidowski, R. Gebhart, H. Ferreira, I. Kuprov, J. Pfaendtner, G. Drobny, "Combining Molecular and Spin Dynamics Simulations with Solid-State NMR to Study Amphiphilic Lysine-Leucine Repeat Peptide Aggregates," *J. Phys. Chem. B* **2019**, 123(51), 10915-10929. DOI: 10.1021/acs.jpcb.9b09245
86. M. Bonomi, G. Bussi, C. Camiloni, G. Tribello, et al. (incl. J. Pfaendtner), "Promoting transparency and reproducibility in enhanced molecular simulations," *Nature Methods* **2019**, 16, 670-673. DOI: 10.1038/s41592-019-0506-8
85. B. Li, P. Jain, J. Ma, J. Smith[1], Z. Yuan, H.C. Hung, Y. He, X. Lin, K. Wu, J. Pfaendtner, S. Jiang, "Trimethylamine *N*-oxide–derived zwitterionic polymers: A new class of ultralow fouling bioinspired materials," *Sci. Adv.* **2019**, 5(6), eaaw9562. DOI: 10.1126/sciadv.aaw9562.

84. S. Xie, C. Jia, A. Prakash[1], M.I. Palafox, J. Pfaendtner, H. Lin, "Generic Biphasic Catalytic Approach for Producing Renewable Diesel from Fatty Acids and Vegetable Oils," *ACS Catal.* **2019**, 9(4), 3753-3763. DOI: 10.1021/acscatal.9b00215
83. W. Beckner[1], J. Pfaendtner, "Fantastic Liquids and Where to Find Them: Optimizations of Discrete Chemical Space," *J. Chem. Inf. Model.* **2019**, 59(6), 2617-2625. DOI: 10.1021/acs.jcim.9b00087
82. M. Mao[1], J. Sampath[2], K.G. Sprenger[1], G. Drobny, J. Pfaendtner, "Molecular Driving Forces in Peptide Adsorption to Metal Oxide Surfaces," *Langmuir* **2019**, 35(17), 5911-5920. DOI: 10.1021/acs.langmuir.8b01392
81. C.D. Fu[1], Y. He, J. Pfaendtner, "Diagnosing the Impact of External Electric Fields Chemical Kinetics: Application to Toluene Oxidation and Pyrolysis," *J. Phys. Chem A* **2019**, 123(14), 3080-3089. DOI: 10.1021/acs.jpca.8b11780
80. E.L. Buckle[*], A. Prakash[1*], M. Bonomi, J. Sampath[2], J. Pfaendtner, G.P. Drobny, "A Solid-State NMR and MD Study of the Structure of the Statherin Mutant SNa15 on Mineral Surfaces," *J. Am. Chem. Soc.* **2019**, 141(5), 1998-2011. DOI: 10.1021/jacs.8b10990
79. D. Verreault, S. Alamdari[1], S. Roeters, R. Pandey, J. Pfaendtner, T. Weidner, "Ice-binding site of surface-bound type III antifreeze protein partially decoupled from water," *Phys. Chem. Chem. Phys.* **2018***,* 20(42), 26926-26933. DOI: 10.1039/C8CP03382J
78. K. Oleson, K.G. Sprenger[1], J. Pfaendtner, D.T. Schwartz, "Inhibition of the Exoglucanase Cel7A by a Douglas-Fir-Condensed Tannin," *J. Phys. Chem. B* **2018**, 122 (37), 8665–8674 DOI: 10.1021/acs.jpcb.8b05850
77. A. Prakash[1], C.D. Fu[1], M. Bonomi, J. Pfaendtner, "Biasing Smarter, Not Harder, By Partitioning Collective Variables Into Families in Parallel Bias Metadynamics," *J. Chem. Theory Comput.* **2018**, 14(10), 4985–4990. DOI: 10.1021/acs.jctc.8b00448
76. A. Mafi, J.N. Kizhakkedathu, J. Pfaendtner, K.C. Chou, "Design of Polyphosphate Inhibitors: a Molecular Dynamics Investigation on Polyethylene-glycol-linked Cationic Binding Groups," *Biomacromolecules* **2018**, 19(4), 1358-1367. DOI: 10.1021/acs.biomac.8b00327
75. W. Beckner[1], C.M. Mao[1], J. Pfaendtner, "Statistical Models Are Able to Predict Ionic Liquid Viscosity Across a Wide Range of Chemical Functionalities and Experimental Conditions," *Mol. Sys. Des. Eng.* **2018**, 3, 253-263. DOI:10.1039/C7ME00094D [Invited contribution to emerging investigator issue]
74. A. Prakash[1], M. Baer, C.J. Mundy, J. Pfaendtner, "Peptoid backbone flexibility dictates its interaction with water and surfaces: A molecular dynamics investigation," *Biomacromolecules* **2018**, 19(3), 1006-1015. DOI: 10.1021/acs.biomac.7b0181
73. C.D. Fu[1], L.F.L. Oliveira[2], J. Pfaendtner, "Lifting the Curse of Dimensionality on Enhanced Sampling of Reaction Networks with Parallel Bias Metadynamics," *J. Chem. Theory Comput.* **2018**, 14(5), 2516-2525. DOI: 10.1021/acs.jctc.7b01289
72. L.F.L. Oliveira[2], C.D. Fu[1], J. Pfaendtner, "Density functional tight-binding and infrequent metadynamics can capture entropic effects in intramolecular hydrogen transfer reactions," *J. Chem. Phys.* **2018**, 148, 154101. DOI:10.1063/1.5021359

71. A. Prakash[1], K.G. Sprenger[1], J. Pfaendtner, "Essential slow degrees of freedom in protein-surface simulations: A metadynamics investigation," *Biochem. Biophys. Res. Commun.* **2018**, 498, 274-281. DOI:10.1016/j.bbrc.2017.07.066
70. K.G. Sprenger[1], A. Prakash[1], G. Drobny, J. Pfaendtner, "Investigating the Role of Phosphorylation in the Binding of Silaffin Peptide R5 to Silica with Molecular Dynamics Simulations," *Langmuir* **2018**, 34, 1199-1207. DOI: 10.1021/acs.langmuir.7b02868. [Invited article for Emerging Investigators Issue]
69. M.A. Donovan, H. Lutz, Y.Y. Yimer[2], J. Pfaendtner, M. Bonn, T. Weidner, "LK peptide side chain dynamics at interfaces are independent of secondary structure," *Phys. Chem. Chem. Phys.* **2017**,19, 28507-28511. DOI: 10.1039/C7CP05897G
68. S.R. Summers, K.G. Sprenger[1], J. Pfaendtner, J. Marchant, M.F. Summers, J.L. Kaar, "Mechanism of Competitive Inhibition and Destabilization of *Acidothermus cellulolyticus* Endoglucanase 1 by Ionic Liquids," *J. Phys. Chem. B* **2017**, 121(48), 10793-10803. DOI: 10.1021/acs.jpcb.7b08435
67. J.K. Smith[1], S. Jiang, J. Pfaendtner, "Redefining the Protein–Protein Interface: Coarse Graining and Combinatorics for an Improved Understanding of Amino Acid Contributions to the Protein–Protein Binding Affinity," *Langmuir* **2017**, 33(42), 11511–11517. DOI: 10.1021/acs.langmuir.7b02438
66. A. Prakash[1], J. Pfaendtner, J. Chun, C.J. Mundy, "Quantifying the Molecular-Scale Aqueous Response to the Mica Surface," *J. Phys. Chem. C* **2017**, 121(34), 18496–18504. DOI: 10.1021/acs.jpcc.7b03229
65. H. Lu, Y. Yimer[2], R. Berger, M. Bonn, J. Pfaendtner, T. Weidner, "Thiolated Lysine-Leucine Peptides Self-Assemble into Biosilica Nucleation Pits on Gold Surfaces," *Adv. Mater. Interfaces* **2017**, 4(16), 1700399. DOI: 10.1002/admi.201700399
64. D. Beck, J. Pfaendtner, J. Carothers, V. Subramanian, "Data Science for Chemical Engineers," *Chem. Eng. Prog.* **2017**, 113(2), 21-26
63. S. Tan, T. Xia, Y. Shi, J. Pfaendtner, Z. Shuangliang, Y. He, "Enhancing the Oxidation of Toluene with External Electric Fields: A Reactive Molecular Dynamics Study," *Sci. Rep.* **2017**, 7, 1710, DOI: 10.1038/s41598-017-01945-4
62. K.G. Sprenger[1], J. Smith[1], R. Liao, A. Joseph, E.A. Nance, J. Pfaendtner, "Determining dominant driving forces affecting controlled protein release from polymeric nanoparticles," *Biointerphases* **2017**, 12(2), 02D412. DOI: 10.1116/1.4983154
61. K.G. Sprenger[1], J.G. Plaks, J. Kaar, J. Pfaendtner, "Elucidating sequence and solvent specific design targets to protect and stabilize enzymes for biocatalysis in ionic liquids," *Phys. Chem. Chem. Phys*. **2017**, 19, 17426-17433. DOI: 10.1039/C7CP03013D
60. K.G. Sprenger[1], K. Palunas[3], T. Weidner, J. Pfaendtner, "Effect of an Ionic Liquid/Air Interface on the Structure and Dynamics of Amphiphilic Peptides," *J. Mol. Liq.* **2017**, 236, 404-413, DOI: 10.1016/j.molliq.2017.04.027
59. H. Lutz, V. Jaeger[1], L. Schmüser, M. Bonn, J. Pfaendtner, T. Weidner, "The Structure of the Diatom Silaffin Peptide R5 within Freestanding Two-Dimensional Biosilica Sheets," *Angew. Chem., Int. Ed.* **2017**, 56(28), 8277-8280. DOI: 10.1002/anie.201702707

58. C.D. Fu[1], L.F.L. Oliveira[2], J. Pfaendtner, "Assessing Generic Collective Variables for Determining Reaction Rates in Metadynamics Simulations," *J. Chem. Theory Comput.* **2017**, 13(3), 968-973. DOI: 10.1021/acs.jctc.7b00038
57. X. Ma, S. Zhang, F. Jiao, C. Newcomb, Y. Zhang, A. Prakash[1], Z. Liao, M. Baer, C. Mundy, J. Pfaendtner, A. Noy, C. Chen, J. De Yoreo, "Tuning crystallization pathways through sequence-engineering of biomimetic polymers," *Nat. Mater.* **2017**, 16, 767-774. DOI: 10.1038/nmat4891
56. B. Hough[1], D.A.C. Beck, D.T. Schwartz, J. Pfaendtner, "Application of machine learning to pyrolysis reaction networks: reducing model solution time to enable process optimization," *Comput. Chem. Eng.* **2016***,* 104(2), 56-63*.* DOI: 10.1016/j.compchemeng.2017.04.012
55. C.D. Fu[1], L.F.L. Oliveira[2], J. Pfaendtner, "Determining Energy Barriers and Selectivities of a Multi-Pathway System with Infrequent Metadynamics," *J. Chem. Phys.* **2017**, 146(1), 014108. DOI: http://dx.doi.org/10.1063/1.4971800
54. H. Lutz, V. Jaeger[1], M. Bonn, J. Pfaendtner, T. Weidner, "Acetylation dictates the morphology of nanophase biosilica precipitated by a 14-amino acid leucine-lysine peptide," *J. Peptide Sci.* **2017**, 23(2), 141-147. DOI: 10.1002/psc.2960
53. V. Jaeger[1], J. Pfaendtner, "Destabilization of Human Serum Albumin by Ionic Liquids Studied Using Enhanced Molecular Dynamics Simulations," *J. Phys. Chem. B* **2016**, 120(47), 12079-12087. DOI: 10.1021/acs.jpcb.6b09410
52. W.A. Beckner[1], Y. He, J. Pfaendtner, "Chain Flexibility in Self-Assembled Monolayers Affects Protein Adsorption and Surface Hydration, a Molecular Dynamics Study," *J. Phys. Chem. B* **2016***,* 120(40), 10423-10432. DOI: 10.1021/acs.jpcb.6b05882
51. H. Tung[1], J. Pfaendtner, "Kinetics and mechanism of ionic-liquid induced protein unfolding: Application to the model protein HP35," *Mol. Syst. Des. Eng.* **2016**, 1, 382-390. DOI: 10.1039/C6ME00047A
50. B. Hough[1], D.T. Schwartz, J. Pfaendtner, "Detailed kinetic modeling of lignin pyrolysis for process optimization," *Ind. Eng. Chem. Res.* **2016**, 55(34), 9147-9153. DOI: 10.1021/acs.iecr.6b02092
49. R. Pandey, K. Usui, R.A. Livingstone, S.A. Fischer[2], J. Pfaendtner, E.H.G. Backus, Y. Nagata, J. Fröhlich-Nowoisky, L. Schmüser, S. Mauri, J.F. Scheel, D.A. Knopf, U. Pöschl, M. Bonn, T. Weidner, "Ice Nucleating Bacteria Control Order and Dynamics of Interfacial Water," *Sci. Adv.* **2016**, 2(4), e1501630. DOI: 10.1126/sciadv.1501630
48. K.G. Sprenger[1], Y. He, J. Pfaendtner, "Probing how defects in self-assembled monolayers affect peptide adsorption with molecular simulation," in *Molecular Modeling and Simulation*, **2016**, 21-35, R. Q. Snurr, C. Adjiman, D. Kofke, Eds. DOI: 10.1007/978-981-10-1128-3_2
47. K.G. Sprenger[1], J. Pfaendtner, "Strong Electrostatic Interactions Lead to Entropic Stabilization of Peptides on Surfaces," *Langmuir* **2016**, 32 (22), 5690–5701. DOI: 10.1021/acs.langmuir.6b01296
46. C. Krumm, J. Pfaendtner, P.J. Dauenhauer, "Millisecond Pulsed Films Unify the Mechanisms of Cellulose Fragmentation," *Chem. Mater.* **2016**, 28(9), 3108-3114. DOI: 10.1021/acs.chemmater.6b00580
45. D. Beck, J.M. Carothers, V. Subramanian, J. Pfaendtner, "Data science: Accelerating innovation and discovery in chemical engineering," *AIChE J.* **2016**, 62(5), 1402-1416. DOI: 10.1002/aic.15192

44. M. Donovan, Y. Yimmer, J. Pfaendtner, E. Backus, M. Bonn, T. Weidner, "Ultrafast reorientational dynamics of leucine at the air-water interface," *J. Am. Chem. Soc.* **2016**, *138* (16), 5226–5229. DOI: 10.1021/jacs.6b01878
43. K.G. Sprenger, A. Choudhury, J.L. Kaar, J. Pfaendtner, "Lytic Polysaccharide Monooxygenases ScLPMO10B and ScLPMO10C Are Stable in Ionic Liquids as Determined by Molecular Simulations," *J. Phys. Chem. B* **2016**, 120(16), 3863-3872. DOI: 10.1021/acs.jpcb.6b01688
42. K. Fleming[1], P. Tiwary, J. Pfaendtner, "New Approach for Investigating Reaction Dynamics and Rates with Ab Initio Calculations," *J. Phys. Chem. A* **2015**, 120(2), 299-305. DOI: 10.1021/acs.jpca.5b10667 [ACS Editors' Choice]
41. T. Bereau, W.F. Drew Bennett, J. Pfaendtner, M. Deserno, M. Karttunen, "Folding and insertion thermodynamics of the transmembrane WALP peptide," *J. Chem. Phys.* **2015**, 143, 243127. DOI: 10.1063/1.4935487
40. J. Pfaendtner, M. Bonomi, "Efficient sampling of high-dimensional free-energy landscapes with Parallel Bias Metadynamics," *J. Chem. Theory Comput.* **2015**, 11(11), 5062-5067. DOI: 10.1021/acs.jctc.5b00846
39. H. Lutz, V.W. Jaeger[1], R. Berger, M. Bonn, J. Pfaendtner, T. Weidner, "Biomimetic Growth of Ultrathin Silica Sheets Using Artificial Amphiphilic Peptides," *Adv. Mater. Interfaces* **2015**, 2(17), e1500282. DOI: 10.1002/admi.201500282
38. P. de la Iglesia, V.W. Jaeger[1], Y. Xi, J. Pfaendtner, L. D. Pozzo, "Structure Characterization and Properties of Metal-Surfactant Complexes Dispersed in Organic Solvents," *Langmuir* **2015**, 31(33), 9006-9016. DOI: 10.1021/acs.langmuir.5b02071
37. Z. Levine, S.A. Fischer[2], J.E. Shea, J. Pfaendtner, "Trp-Cage Folding on Organic Surfaces," *J. Phys. Chem. B* **2015**, 119(3), 10417-10425. DOI: 10.1021/acs.jpcb.5b04213
36. R. Elder, J. Pfaendtner, A. Jayaraman, "Effect of hydrophobic and hydrophilic surfaces on the stability of double-stranded DNA," *Biomacromolecules* **2015**, 16(6), 1862-1869. DOI: 10.1021/acs.biomac.5b00469
35. K.G. Sprenger[1], V.W. Jaeger[1], J. Pfaendtner, "The General AMBER Force Field (GAFF) Can Accurately Predict Thermodynamic and Transport Properties of Many Ionic Liquids," *J. Phys. Chem. B* **2015**, 119(18), 5882-5895. DOI: 10.1021/acs.jpcb.5b00689
34. P. Burney[1], E. M. Norwald, K. Hickman[3], J.L. Kaar, J. Pfaendtner, "Molecular dynamics investigation of the ionic liquid/enzyme interface: Application to engineering enzyme surface charge," *Proteins* **2015***,* 83(4), 670-680. DOI: 10.1002/prot.24757
33. G. Newbloom, S. Hoffmann[1], A. West, M. Gile[3], P. Sista, H. Cheung, C. Luscombe, J. Pfaendtner, L.D. Pozzo, "Solvatochromism and Conformational Changes in Fully Dissolved Poly(3-alkylthiophene)s," *Langmuir* **2015**, 31(1), 458-468*.* DOI: 10.1021/la503666x
32. V. Jaeger[1], P. Burney[1], J. Pfaendtner, "Comparison of Three Ionic Liquid Tolerant Cellulases by Molecular Dynamics," *Biophys. J.* **2015**, 108(4), 880-892. DOI: 10.1016/j.bpj.2014.12.043
31. K. Fleming[1], J. Matthei, J. Pfaendtner, "A new graduate level seminar to prepare students for the next step in their career," *Chem. Eng. Educ.* **2015**, 49(1) 29-37.
29. J.E. Baio, A. Zane, V. Jaeger[1], A.M. Roehrich, H. Lutz, J. Pfaendtner, G.P. Drobny, T. Weidner, "Diatom mimics: directing the formation of biosilica nano-particles by controlled folding of lysine-leucine peptides," *J. Am. Chem. Soc.* **2014**, 136(43), 15134-15137. DOI: 10.1021/ja5078238

28. S. Zheng[2], J. Pfaendtner, "Enhanced sampling of chemical and biochemical reactions with metadynamics," *Mol. Simulat.* **2015**, 41(1-3), 55-72. DOI: 10.1080/08927022.2014.923574 [invited review article]
27. S. Zheng[2], J. Pfaendtner, "Car–Parrinello Molecular Dynamics + Metadynamics Study of High-Temperature Methanol Oxidation Reactions Using Generic Collective Variables," *J. Phys. Chem. C* **2014**, 118(20), 10764-10770.
26. Z. Jarin[3], J. Pfaendtner, "Ionic Liquids Can Selectively Change the Conformational Free-Energy Landscape of Sugar Rings," *J. Chem. Theory Comput.* **2014**, 10(2), 507-510.
25. P. Burney[1], N. White, J. Pfaendtner, "Structural Effects of Methionine Oxidation on Isolated Subdomains of Human Fibrin D and αC regions," *PLoS One* **2014**, 9(1), e68981.
24. A.D. Paulsen, B.R. Hough[1], C.L. Williams, A.R. Teixeira, D.T. Schwartz, J. Pfaendtner, P.J. Dauenhauer, "Fast Pyrolysis of Wood Particles: Spatiotemporally-Resolved Diffuse Reflectance in situ Spectroscopy of Particles (STR-DRiSP)," *ChemSusChem* **2014**, 7(3), 765-776.
23. K. L. Fleming, J. Pfaendtner, "Characterizing the catalyzed hydrolysis of β-1,4 glycosidic bonds using DFT," *J. Phys. Chem. A* **2013**, 117(51), 14200-14208.
22. M. Deighan, J. Pfaendtner, "Exhaustively Sampling Peptide Adsorption with Metadynamics," *Langmuir* **2013**, 29(25), 7999-8009.
21. A. White, A. Keefe, J.R. Ella-Menye, A. Nowinski, Q. Shao, J. Pfaendtner, S. Jiang, "Free Energy of Solvated Salt Bridges: A Simulation and Experimental Study," *J. Phys. Chem. B* **2013**, 117(24), 7254-7259.
20. V. Jaeger[1], J. Pfaendtner, "Structure, Dynamics and Activity of Xylanase Solvated in Binary Mixtures of Ionic Liquid and Water," *ACS Chem. Biol.* **2013**, 117(9), 2662-2670.
19. P. Burney[1], J. Pfaendtner, "Structural and dynamic features of *Candida rugosa* Lipase1 in Water, Octane, Toluene, and Ionic Liquids BMIM-PF_6 and BMIM-NO_3," *J. Phys. Chem. B* **2013**, 117(9), 2662-2670.
18. M. Deighan[1], M. Bonomi, J. Pfaendtner, "Efficient Simulation of Explicitly Solvated Proteins in the Well-Tempered Ensemble," *J. Chem. Theory Comput*. **2012**, 8, 2189-2192.
17. J. Pfaendtner, N. Volkmann, D. Hanein, P. Dalhaimer, T.D. Pollard, G.A. Voth, "Key Structural Features of the Actin Filament Arp2/3 Complex Branch Junction Revealed by Molecular Simulation," *J. Mol. Biol*. **2012**, 416 (*1)*, 148-161
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14. J. Pfaendtner, E. Lyman, T.D. Pollard, G.A. Voth., "Structure and dynamics of the actin filament," *J. Mol. Biol.* **2010**, 396 (2), 252-263. [*journal cover*]
13. Z. Zhang, J. Pfaendtner, A. Grafmüller, G.A. Voth, "Defining coarse-grained representations of large biomolecules and biomolecular complexes from elastic network models," *Biophys. J.* **2009**, 97(8), 2327-2333.
12. J. Pfaendtner, G.A. Voth, "Molecular Dynamics Simulation and Coarse-grained Analysis of the Unactivated Arp2/3 Complex," *Biophys. J.* **2008**, *95* (11), 5324-5333.

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5. J. Pfaendtner, L. J. Broadbelt, "Contra-thermodynamic Behavior in Intermolecular Hydrogen Transfer of Alkylperoxy Radicals, ROO· + R'H," *ChemPhysChem* **2007**, *8* (13), 1969-1978.
4. J. Pfaendtner, X. Yu, L. J. Broadbelt, "The 1D Hindered Rotor Approximation," *Theor. Chem. Acc*. **2007**, *118* (5-6), 881-898.
3. J. Pfaendtner, L.J. Broadbelt, "Elucidation of Structure-Reactivity Relationships in Hindered Phenols Via Quantum Chemistry and Transition State Theory," *Chem. Eng. Sci*. **2007**, *62* (18-20), 5232-5239.
2. J. Pfaendtner, X. Yu, L.J. Broadbelt, "Quantum Chemical Investigation of Low-Temperature Intramolecular Hydrogen Transfer Reactions of Hydrocarbons," *J. Phys. Chem. A* **2006**, *110* (37), 10863-10871.
1. L.J. Broadbelt, J. Pfaendtner, "Lexicography of Kinetic Modeling of Complex Reaction Networks," *AIChE J*. **2005**, *51* (8), 2112-2121.

Parts of books (chapters in edited books)

4. J. Pfaendtner, "Metadynamics to Enhanced Sampling in Biomolecular Simulations", (*invited contribution*) in *"Molecular Modeling of Proteins"*, 2019, in press
3. K.G. Sprenger[1], J. Pfaendtner, "Using molecular simulation to study biocatalysis in ionic liquids"*, (invited contribution),* in Methods in Enzymology, 2016, 577, 419-441, ed. Gregory A. Voth. DOI: 10.1016/bs.mie.2016.05.020
2. A. Barducci, J. Pfaendtner, M. Bonomi, "Tackling sampling challenges in biomolecular simulations", *in press*, [invited book chapter in "Molecular Modeling of Proteins, 2nd edition"]
1. J. Pfaendtner, Chemical and Biochemical Kinetics and Macrokinetics , in *Chemical Engineering and Chemical Process Technology*, [Eds. Ryzhard Pohorecki, John Bridgwater, Rafiqul GANI], in *Encyclopedia of Life Support Systems (EOLSS),* 2009, Developed under the Auspices of the UNESCO, EOLSS Publishers, Oxford, UK.

V. TEACHING

V-I. INDIVUDAL INSTRUCTION

Former Postdoctoral or Graduate Advisees

Dr. Kayla Sprenger [Ph.D. Chemical Engineering 2017]
Garett Davidson [nonthesis masters in ChemE 2017]
Dr. Yeneneh Yimer [postdoc 2014-2106]
Dr. Sean Fischer [postdoc during 2014]
Shaohui Zheng [postdoc from 2012-2015]
Dr. Blake Hough [Ph.D. Chemical Engineering 2016] (co-advised with Dan Schwartz)
Dr. Kelly Fleming [Ph.D. Chemical Engineering 2015]
Dr. Vance Jaeger [Ph.D. Chemical Engineering 2015]
Dr. Michael Deighan [Ph.D. Chemical Engineering 2014]
Dr. Patrick Burney [Ph.D. Chemical Engineering 2014]
Ms. Stephanie Hoffman [thesis masters in ChemE 2014]
Mr. Moses Cho [nonthesis masters in ChemE 21013]
Dr. Cristina Russo [postdoc from 2010-2011]

Current Postdoctoral Advisees

Dr. Luiz Oliveira

Current Graduate Advisees

Sarah Alamdari, NSF NRT trainee, NSF GRFP | Wesley Beckner, NSF NRT trainee | Luke Gibson, NSF NRT trainee | Christopher Fu, NSF IGERT trainee | Moke Mao | Christopher Nyambura (co-advised with Elizabeth Nance) | Tai-Yu Pan | Arushi Prakash (co-advised with Christopher J. Mundy, PNNL) | Khushmeen Sakloth | Joshua Smith (co-advised with Shaoyi Jiang) | Kejia Wu

Former and Current Undergraduate Researchers, REU students

Melissa Gile, Peter Englund, Christopher Fu, Nikita Grover, Katie Hoffman, Samuel Hwang, Miwako Ito, Zachary Jarin, Christof Krumm, Brittany Lasher, Ryan Ly, Albert Ng, Kovas Palunas, Eric Poehlman, Stephanie Robinson, Parashara Shamaparasad, Suzanne Silva, Rachel Scholes, Jake Turk, Jude Tunyi, Kayla Vanous, Allen Wong

V-II. CLASSROOM INSTRUCTION

All courses taught at University of Washington

Course	Quarter & Year Taught	Instructor Ranking[1]	
		"Instructor's effectiveness in teaching the course"	**"Instructor's contribution to the course"**
CHEM E 545 (*data science methods*)	WI17	4.6 (4.4)	4.6 (4.5)
CHEM E 435 (*mass transfer and separations)*	AU14	4.8 (5.0)	4.7 (4.9)
	AU15	4.6 (4.9)	4.8 (5.1)
	AU16	3.4 (3.8)	3.7 (4.1)
CHEM E 465 (*reactor design)*	AU10	4.6 (4.8)	4.8 (5.0)
	AU11	4.7 (5.1)	4.6 (4.9)

	AU12	4.8 (5.2)	4.9 (5.3)
	AU13	4.9 (5.1)	4.8 (5.0)
CHEM E 375 *(computer skills)*	WI10	4.5 (4.2)	4.5 (4.3)
	WI11	4.7 (4.5)	4.9 (4.7)
	WI12	4.9 (4.5)	4.9 (4.5)
	WI13	4.8 (4.6)	4.7 (4.5)
	WI14	4.9 (4.7)	4.9 (4.7)
	WI15	4.9 (4.6)	4.9 (4.6)
	WI16	4.8 (4.4)	4.8 (4.4)
CHEM E 437[2] *(senior lab)*	WI11	4.7 (4.5)	4.5 (4.4)
	WI12	3.6 (3.9)	3.7 (3.9)
CHEM E 485 *(senior design I)*	WI13	4.9 (5.0)	4.8 (5.2)
	WI14	4.9 (4.9)	4.7 (4.8)
CHEM E 599 *(multiscale modeling)*	SP10	4.8 (4.7)	4.5 (4.3)

[1]0-5 scale; UW adjusted means (based on certain course criteria such as difficulty) in parentheses

[2]co-taught 4 sections with Lilo Pozzo (UW CHEM E)

V-III. WORKSHOPS

- Organizer (with William H. Green, MIT) for Telluride Science Research Center Workshop on De Novo Prediction of Chemical Reaction Networks (July 2016)
- Organizer Committee Member for ISCRE24 (International Symposium of Chemical Reaction Networks) (June 2016)
- Organizer and PI (Cameron Abrams, Drexel University, co-PI) for NSF workshop on Multiscale Modeling and Simulation (September 2012)

VI. PROFESSIONAL SERVICE

Departmental and University Contributions

- Co-Chair, UW QuantumX, 2018-2020
- Chair, UW BioEngineering Chair Search Advisory Committee, 2019
- Associate Vice Provost for Research Computing, 2018 – present
- Graduate Program Director, 2014 – 2018 (*break 9/17 – 6/18 for sabbatical*)
- UW Clean Energy Institute Faculty Advisory Board, 2017-19
- COE ad hoc Committee on leadership development, 2016-17
- UW Provost Leadership Excellence Program, 2015-2017
- UW Husky 100 Advisory Board, 2016-17
- Center for Teaching and Learning "Senior Fellow", 2016-18
- CAMCET Building Visioning and Scoping Faculty Advisory – Education Thrust, 2015-16
- UW Husky 100 reviewer, 2015-16
- Creator and faculty advisor for new student High Performance Computing Club, 2015-present
- UW "Board of Environmental Health & Safety" UW President Faculty Advisory Committee, 2015-2017
- UW Orientation "Meet a Professor" parent/faculty speaker, 2015

- UW Distinguished Teaching Award selection panel, 2015-2016
- UW "Husky Experience" Faculty Advisory Committee to Vice Provost for Student Affairs, 2015
- UW COE Underclassmen Planning Committee, 2015
- Panelist for "Meet Greet Teach" event in UW College of Environment, 2015
- Conceived and executed new departmental "young scholars seminar series", 2011-2015
- ChemE Department Faculty Search Committee, 2011-2014 [search co-chair 2013-14]
- Civil and Environmental Engineering Search Committee 2013-2014
- Department Computer Committee, 2009-2017
- Responsible for all aspects of department graduate recruiting weekend(s), 2011-2014
- University Steering Committee for Campus High Performance Computing (HYAK), 2012-present
- Faculty Advisor for "Biodiesel Cooperative" (Undergrad Student Organization), 2012-2016
- Faculty Advisor for Tau Beta Pi (Undergrad Engineering Honor Society), 2012-2016
- Faculty Advisor for ACES (Graduate Student Professional Organization), 2009-2012, 2014-present
- Organizer of Department Seminar Series, 2009-2012
- Guest lecturer, 6 Molecular & Engineering Science undergraduate/graduate courses, 2009-2015
- Panelist at UW ADVANCE CAREER workshop, 2012, 2014
- Panelist at UW NSF GRF workshop, 2012-15, 17
- Conceived and executed "grad school info night" for ChemE undergrads, 2010-2012
- Steering committee for new Molecular Engineering PhD program, 2011-2012
- Conceived and executed graduate reading group with diversity focus, 2011
- Conceived and executed "preparing for ChemE faculty careers" seminar, 2010

Session Chair and Meeting Organization

- AIChE Area 21 (CoMSEF) Vice Chair, 2017-2019
- ISCRE 24 Scientific Advisory Committee, 2015-2016
- AIChE Computational Science and Molecular Engineering Forum "Liason Director", 2013-2015
- AIChE Area 20B (Catalysis and Reaction Engineering) Programming Chair, 2012-2014
- Organizer and PI for NSF Pan American Studies Institute on Multiscale Modeling, 2012
- Session Chair or Co-Chair at the 2013, 2014, 2015 Annual Meetings (1-2 sessions/year)
- Session Chair or Co-Chair at the 2012 AIChE Annual Meeting, Pittsburgh, PA (3 sessions)
- Session Chair or Co-Chair at the 2011 AIChE Annual Meeting, Minneapolis, MN (4 sessions)
- Session Chair or Co-Chair at the 2010 AIChE Annual Meeting, Salt Lake City, UT (3 sessions)

Scientific Reviews and Panels

2019-2021: Advisory committee member for PNNL's Energy Storage Materials Initiative
2018: Ad hoc reviewer for NSF and DOE
2017: Ad hoc reviewer for NSF and DOE
2016: Reviewer for 1 NSF panel, ad hoc review for Belgium Science Foundation, DOE and AFOSR
2015: Reviewer on 3 NSF panels, Ad hoc review for Shell-NWO/FOM (Netherlands) grant proposals
2014: Reviewer on 3 NSF panels
2013: Reviewer on 2 NSF panels
2012: Reviewer on 5 NSF panels

2011: Reviewer on 4 NSF panels
2011: Ad hoc reviewer for ACS (PRF and ND programs)
2009-10: Ad hoc reviewer for INDO-US Science and Technology Forum Workshops

Journal Referee and Editorial

- Associate Editor for *npj Computational Materials* (May 2020–present)
- Guest Editor for ACS Journal of Physical Chemistry Virtual Special Issue on Machine Learning in Physical Chemistry (2020)
- Editorial Advisory Board of the ACS Journal of Chemical & Engineering Data (1/2019–12/2021)
- Co-editor of special issue of Current Opinion in Chemical Engineering – Frontiers in Chemical Engineering: Molecular Modeling (March 2019)

Journal referee: ACS Catalysis, AIChE Journal, Applied Catalysis B: Environmental, Applied Physics A, Biochemistry, BioEnergy Research, Biophysical Journal, Biotechnology & Bioengineering, ChemPhysChem, Computers and Chemical Engineering, Computational and Mathematical Methods in Medicine, Computer Physics Communications, Energy & Fuels, Environmental Science & Technology, Enzyme and Microbial Technology, European Biophysics Journal, IE&CR, Journal of the American Chemical Society, Journal of Chemical Information and Modeling, Journal of Molecular Graphics & Modeling, Journal of Molecular Liquids, Journal of Physical Chemistry, PNAS, PLOS Computational Biology, Process Biochemistry, Protein Engineering Design & Selection, PLoS One, Soft Matter, Theoretical Chemistry Accounts, Thermochimica Acta

Industrial/Corporate

- 2018: Consulting on technology for catalysis of rocket fuel for space propulsion applications
- 2010 – 2014, 2017: Consulting in research on kinetics of food chemistry for a Fortune 500 company specializing in food and beverage

VII. RESEARCH FUNDING AS PI OR CO-PI SINCE 2007

NSF International Research Fellows Program [9/1/2007–8/31/2009]
Biomass-Derived Fuels: Modeling and Simulation of Enzymatic Processes
Role: PI Funding: $156,000

NSF BRIGE Program [9/1/2010–8/31/2013]
Understanding Protein-Surface Interactions Through Multiscale Modeling: Application to Biofuel Cells
Role: PI Funding: $187,172

NSF CCLI (Lab / Education Grant) [9/1/2010-8/31/2013]
A Consolidated Chemical Engineering Laboratory with a Focus on Bioenergy
Role: Co-PI, PI: L.D. Pozzo, UW Funding: $199,360

NSF EAGER [1/15/2011–1/14/2012]
COLLABORATIVE RESEARCH: Pyrolysis of Cellulose Intermediate Liquids: Automated Mechanism Development and Experimental Characterization
Role: Co-P, PI: Paul Dauenhauer, UMASS Funding: $79,999 (total)

NSF Pan American Advanced Studies Institute [12/1/2011–11/30/2012]

Molecular-Based Multiscale Modeling and Simulation; Montevideo, Uruguay; September 1-14, 2012
Role: PI Co-PI: Cameron Abrams, Drexel Funding: $100,000

NSF CAREER [3/15/2012–3/14/2017]
Computational Enzymology of Non-Aqueous Biocatalysis–Application to Biomass Pretreatment$484,750

NSF Catalyzing New International Collaborations [5/1/2012–4/30/2013]
Integrating Multiscale Modeling With Protein-Surface Experiments Funding: $17,262

AFOSR Core Funding [4/1/2012–3/31/2015]
Automated Discovery of Energetic Ionic Liquid Chemistry: Reaction Topology, Thermochemistry and Kinetics
Role: PI Funding: $360,000

ACS PRF Doctoral New Investigator Program [9/1/2012–8/31/14]
Theoretical Considerations of Conjugated Polymer Self-Assembly
Role: PI Funding: $100,000

NSF CBET Core Funding [8/1/0213–7/30/2016]
NSF-DFG: Combining Simulation and Spectroscopy to Determine the Structure and Dynamics of Adsorbed Proteins - Application to Biomass Conversion
Role: PI on NSF side; separate proposal reviewed by DFG to fund Tobias Weidner Funding: $308,000

Exploratory research project with Boeing corporation [8/1/2013–12/31/2015]
Feasibility study for a novel high throughput virtual screening of adhesive/coating compounds
Role: PI Funding: $241,000

UW RRF (internal seed project funding) [9/1/2014–8/31/2015]
Multiscale Modeling Investigation of Peptide Self-Assembly in the Formation of Nanostructures
Role: PI Funding: $34,932

UW STF (student tech fee grant program) [7/1/2015–6/30/2020]
High Performance Computing for All Students Funding: ~$800,000

AFOSR Core Funding [~10/1/2015–9/30/2018]
Interrogating Dynamic, Stochastic and Topological Features of Reaction Networks: Application to Combustion Chemistry
Role: co-PI, PI: Hai Wang, Stanford Funding: $510,000

NSF NNCI: Northwest Nanotechnology Infrastructure (NWNI) [9/15/2015-8/31/2021]
Role: co-PI & lead of computational/modeling thrust for large instrumentation / shared infrastructure grant, PI: Karl Bohringer Funding: $4,500,000 (JP portion: $0)

NSF MRI Program Grant [9/1/2016–8/31/2019]

MRI: Acquisition of a Shared Next-Generation Computer Cluster to Advance Molecular to Nanoscale Science and Engineering
Role: co-PI, PI: Anne McCoy, UW Funding: $622,000

NSF NRT Training Grant [9/1/2016–8/31/2021]
NRT-DESE: Data Intensive Research Enabling Clean Technologies (DIRECT)
Role: PI and director Funding: ~3,800,000, including $800K UW hard cash match

UW Clean Energy Institute Faculty Exploration Grant [9/15/2016–6/15/2017]
Predictive modeling to integrate the physics of battery electrolyte materials with the performance of renewable energy grids
Role: PI Funding: $36,124

PNNL Subcontract [6/15/2015–12/31/2017]
Modeling and Simulation of Peptoids
Role: PI Funding: ~$250,000

NSF MCB Core Funding [6/1/2017–5/31/2020]
A Spectroscopic and Computational Structure-Function Study of Biosilicification Peptides
Role: Co-PI, PI: Gary Drobny Funding: $678,872 (JP portion: $157,528)

NSF CBET Core Funding [9/1/2017–8/31/2021]
Collaborative Research: Combined Computational/Experimental Investigation of Thermochemical Conversion of Xylose at Extreme Conditions
Role: PI, Co-PI: Paul Dauenhauer, UMN Funding: $500,000 (JP portion: $250,000)

NSF CBET Core Funding [9/1/2017–8/31/2021]
Combined molecular simulation and experimental study to discover, predict and control enzyme immobilization in polymeric nanoparticles
Role: PI, Co-PI: Elizabeth Nance, UW Funding: $331,264 (JP portion: $165,632)

DOE BES Core Funding [CPIMS program] 9/15/2018–3/15/2021
Understanding molecular scale chemical transformations at solid-liquid interfaces–computational investigation of interfacial chemistry in electrolytes and charged interfaces
Role: PI (no coPIs) Funding: $488,000

DOE EFRC [8/1/2018–7/31/2022]
The Center for the Science of Synthesis Across Scales (CSSAS)
Role: Co-PI and thrust lead, director and PI: François BaneyxFunding: $10.7M (JP portion ~$550K)

DOE EERE Bioenergy Technology Office [1/1/2019–12/31/2021]
Identifying Performance Advantaged Biobased Chemicals Utilizing Bioprivileged Molecules
Role: Co-PI, PI: Brent Shanks (IA State) Funding: $2.5M (JP portion $450K)

NIH NIDCR R1 [9/15/2017–9/14/2020]
Exploratory Solid State NMR Study of Protein-Metal Oxide Interactions

Role: Co-PI, PI: Gary Drobny Funding: $426K (JP portion $85K)

VIII. PRESENTATIONS

VIII-I. INVITED PRESENTATIONS (SINCE 2009)

- J. Pfaendtner, "Understanding structure-function relationships at the bio/nano interface," University of Houston Chemical Engineering Seminar, Houston, TX, 2020
- J. Pfaendtner, "Understanding structure-function relationships at the bio/nano interface," Oklahoma State University, Stillwater, OK, 2020
- J. Pfaendtner, "Computational design of the bio/nano interface," Xiamen Soft Matter Forum, Xiamen China, 2019
- J. Pfaendtner, "Understanding structure-function relationships at the bio/nano interface," University of Illinois Urbana-Champaign Chemical Engineering Seminar, Champaign, IL, 2019
- J. Pfaendtner, "Understanding structure-function relationships at the bio/nano interface," University of Nebraska Chemical Engineering Seminar, Lincoln, NE, 2019
- J. Pfaendtner, "Peptide adsorption and self-assembly," CECAM meeting on open-source software for enhanced sampling simulations, USI, Lugano CH, 2019
- J. Pfaendtner, "Understanding structure-function relationships at the bio/nano interface," Simon Fraser University Biophysics Seminar, Vancouver CA, 2019
- J. Pfaendtner, "Structural studies of peptide/surface interactions using a high-dimensional enhanced sampling scheme," ACS Annual Spring Meeting, Orlando, FL, 2019
- J. Pfaendtner, "Application of molecular dynamics to discover and quantify reaction pathways," ACS Annual Spring Meeting, New Orleans LA, 2018
- J. Pfaendtner, "Understanding structure-function relationships at the bio/nano interface," State University of New York Buffalo Chemical Engineering Seminar, 2018
- J. Pfaendtner, "Tackling molecular simulation challenges with many slow degrees of freedom," Frontiers of Molecular Modeling & Simulation, 2018, Lake Delavan, Wisconsin
- J. Pfaendtner, "Using Molecular Dynamics to Study Complex Reacting Systems: Discovering Mechanism with Generic Descriptors and Sampling Complex Systems," MACCCR Meeting, 2018, Sandia National Lab
- J. Pfaendtner, "Using Computer Simulations to Understand and Control Chemical Reactions at Extreme Conditions," Washington State University Joint Chemical Engineering & Chemistry Seminar, 2018
- J. Pfaendtner, "Application of molecular dynamics to discover and quantify reaction pathways," ACS Spring National Meeting *Symposium for the 2018 Murphree Award winner*, New Orleans, 2018
- J. Pfaendtner, "Understanding how molecular driving forces give rise to interfacial phenomena of proteins and peptides," University of Wisconsin Chemical & Biological Engineering Seminar, 2018
- J. Pfaendtner, "Enhanced sampling in high dimension," Recent Advances in Modeling Rare Events (RARE) Indo-US modeling symposium, Agra, India, 2017

- J. Pfaendtner, "Applications of molecular modeling and simulation from quantum mechanics to data science," Webinar delivered to PepsiCo global research and development "modeling awareness symposium series," 2017
- J. Pfaendtner, "Applications of Molecular Data Science Tools and Methods to Design of Energy Materials," Energy Internet Research Institute UW/THU joint symposium, Chengdu, China, 2017
- J. Pfaendtner, "Graduate training and research at the nexus of data science and clean energy," Invited keynote lecture, RE^3 Symposium, Louisville, KY 2017
- J. Pfaendtner, "Understanding and controlling protein structure and function at interfaces," University of California–Davis Chemical Engineering Seminar, 2017
- J. Pfaendtner, "Data science tools for biomass pyrolysis – application to thermochemical conversion of lignin," ACS Spring National Meeting, San Francisco, CA, April 2017
- J. Pfaendtner, "Using the Computer to Discover and Control Molecular Scale Driving Forces at the Nano/Bio Interface" Oregon State University Chemical Engineering Seminar, 2017
- J. Pfaendtner, "Using the Computer to Discover and Control Molecular Scale Driving Forces at the Nano/Bio Interface," University of Aarhus (Denmark) Chemistry Seminar, 2017
- J. Pfaendtner, "Discovering and Harnessing Molecular Scale Driving Forces at the Nano/Bio Interface," University of British Columbia Chemistry Seminar, 2017
- J. Pfaendtner, "Using Computer Simulations to Understand and Control Chemical and Biochemical Reactions at Extreme Conditions," Arizona State University Chemical Engineering Seminar, 2016
- J. Pfaendtner, "Computational Tools for Studying Peptide Based Templating of Novel Biomaterials," AIChE Annual Meeting, 2016, San Francisco, CA
- J. Pfaendtner, "Using Molecular Dynamics to Study Complex Reacting Systems," Telluride Science Research Center Workshop on Complex Reacting Systems, 2016
- J. Pfaendtner, "Advanced Methods in Enhanced Sampling," III CCES Workshop and SAMS, Campinas, Brazil, 2016
- J. Pfaendtner, "Discovering Molecular Scale Driving Forces at the Nano/Bio Interface," Columbia University Chemical Engineering seminar, 2016
- J. Pfaendtner, "Multiscale simulations can reveal the effect of ionic liquids on structure and dynamics of biomolecules," AIChE Annual Meeting (CoMSEF Plenary), 2015, Salt Lake City, UT
- J. Pfaendtner, "Using computer simulations to engineer new solvents and interfaces for controlling the behavior of biomolecules," Lehigh University Chemical & Biological Engineering seminar, 2015
- J. Pfaendtner, "Using computer simulations to engineer new solvents and interfaces for controlling the behavior of biomolecules," Zhejiang University Chemical & Biological Engineering seminar, 2015
- J. Pfaendtner, "Using computer simulations to engineer new solvents and interfaces for controlling the behavior of biomolecules," Max Planck Institute for Polymer Science, Mainz, Germany, 2015
- J. Pfaendtner, "Using computer simulations to engineer new solvents and interfaces for controlling the behavior of biomolecules," Princeton University Chemical Engineering seminar, 2015

- J. Pfaendtner, "Using molecular simulations to engineer new solvents and interfaces for controlling the behavior of biomolecules," University of Pennsylvania ChBE seminar, 2014
- J. Pfaendtner, "Engineering the interface between biomolecules, solvents and surfaces using molecular simulation," Georgia Tech ChBE seminar, 2014
- J. Pfaendtner, "Overcoming enhanced sampling challenges in the simulation of proteins on surfaces," University of Delaware Atomic & Molecular Orbital Physics seminar, 2014
- J. Pfaendtner, "Can molecular simulations help us engineer new solvents and interfaces to control the behavior of biomolecules? (hint: yes)," Northwestern University ChBE seminar, 2014
- J. Pfaendtner, "Probing Surface Effects on the Orientation and Conformation of Adsorbed Proteins With Multiscale Simulations," AIChE Annual Meeting, 2013, San Francisco, CA
- J. Pfaendtner, "Discovering the behavior of biomolecules at interfaces and in novel solvents with "bottom up" multiscale modeling," Notre Dame Chemical Engineering seminar, 2013
- J. Pfaendtner, "Discovering the behavior of biomolecules at interfaces and in novel solvents with "bottom up" multiscale modeling," University of California–Santa Barbara BMSD seminar, 2013
- J. Pfaendtner, "Enhanced Sampling of Peptide Adsorption and 2D Self-Assembly with Parallel Tempering Metadynamics," AIChE Annual Meeting, 2012, Pittsburgh, PA
- J. Pfaendtner, "Applications of 'Bottom Up' Multiscale Modeling: Uncovering the Role of Solvents and Surfaces," University of Southern California Mechanical Engineering Seminar, 2012.
- J. Pfaendtner, "Simulation of peptide-surface binding," PLUMED Developer Meeting, Trieste, Italy, 2012.
- J. Pfaendtner, "Coupling molecular simulation of peptide adsorption with experiments: Tackling the sampling challenge," Max Planck Institute for Polymer Science seminar, Mainz Germany, 2012.
- J. Pfaendtner, "Classical molecular dynamics and enhanced sampling of proteins in nonaqueous environments," Max Planck Institute for Biophysics seminar, Frankfurt Germany, 2012.
- J. Pfaendtner, "What can simulations tell us about nonaqueous biocatalysis?" University of Washington Materials Science & Engineering Seminar, 2012.
- J. Pfaendtner, "What can simulations tell us about nonaqueous biocatalysis?" Kansas State University Chemical Engineering Seminar, 2012.
- J. Pfaendtner, "What can simulations tell us about nonaqueous biocatalysis?" Colorado School of Mines Chemical Engineering Seminar, 2012.
- J. Pfaendtner, "What is multiscale modeling and why should you care?" 3M Company, October 2011.
- J. Pfaendtner, "Adventures in the Well-Tempered Ensemble: Getting More by Spending Less," CPMD 2011, Barcelona, Spain, 2011.
- J. Pfaendtner, "Exploring the Thermodynamics of Large-Scale Conformational Change in Macromolecular Systems," University of Washington Physical Chemistry Seminar, 2011.
- J. Pfaendtner, "Multiscale Modeling and Simulation: Application to Protein Self Assembly and Mechanical Properties," Aerodyne Corporation, 2010.
- J. Pfaendtner, "Multiscale Modeling and Simulation: Application to Protein Self Assembly and Mechanical Properties," University of Washington Center for Nanotechnology, 2010.
- J. Pfaendtner, "The Origin of Nucleotide-Dependent Properties In The Actin Filament: A

Multiscale Study," 3rd International Conference on Mechanics of Biomaterials & Tissues, Clearwater Beach, 2009.

VIII-II. CONTRIBUTED PRESENTATIONS (SINCE 2009)

- A. Prakash, K. Sprenger, J. Pfaendtner, "Investigating Biosilification by Silaffin Peptide R5 With Parallel Tempering Metadynamics in the Well-Tempered Ensemble," poster, RARE Meeting, 2017, Agra, India.
- A. Prakash, K. Sprenger, J. Pfaendtner, "Protein Adsorption on Surfaces: The Role of Forcefield and Surface Ions," poster, AIChE Annual Meeting, 2017, Minneapolis, MN.
- A. Prakash, M. Baer, C.J. Mundy, J. Pfaendtner, "What affects peptoid assembly?" poster, Peptoid Summit, 2017, Berkeley, CA.
- A. Prakash, K. Sprenger, J. Pfaendtner, "Exhaustive sampling of protein-surface interactions using classical molecular dynamics and metadynamics," poster, Graduate Women & Postdoc Forum, D.E. Shaw Research, 2017, New York.
- C. Fu, J. Pfaendtner, "Analyzing Reaction Networks and Pathway Kinetics Via Metadynamics Simulations," poster, AIChE Annual Meeting, 2017, Minneapolis, MN.
- C. Fu, J. Pfaendtner, "Analyzing Reaction Networks and Pathway Kinetics Via Metadynamics Simulations," AIChE Annual Meeting, 2017, Minneapolis, MN.
- C. Fu, J. Pfaendtner, "Using Metadynamics to Resolve and Characterize Complex Reactions at the Molecular Scale," AIChE Annual Meeting, 2017, Minneapolis, MN.
- L. D. Gibson, J. Pfaendtner, "Understanding How Mechanical Strain Affects Reactivity of Graphene: A Computational Study," poster, Northwest Theoretical Chemistry Conference, 2017, Pacific Northwest National Laboratory, Richland, WA.
- L. F. L. Oliveira, C. Fu, J. Pfaendtner, "Quantitative Calculation of Reaction Rates of Two Classes of Chemical Reactions by Infrequent Metadynamics Simulations," Materials Research Society Fall Meeting, 2017, Boston, MA.
- A. Prakash, C. Mundy, M. Baer, J. Pfaendtner, "Using Metadynamics to understand the multi-dimensional free energy landscape of peptoid self-assembly," poster, Gordon Research Conference on Computational Chemistry, 2016, Girona, Spain.
- A. Prakash, C. Mundy, M. Baer, J. Pfaendtner, "Electrolytes at the muscovite (001) interface: A molecular dynamics study," 251st American Chemical Society National Meeting, 2016, San Diego, CA.
- Y. Yimer, J. Pfaendtner, "Elucidating Aggregation Mechanisms of Amphiphilic Peptides: A Molecular Dynamics and Metadynamics Simulation Study" Theory & Applications of Computational Chemistry (TACC) Conference, 2016, Seattle, WA
- J. Pfaendtner, "Quantitative Estimates of Chemical Kinetics with Metadynamics," MACCCR Meeting, 2016, Argonne National Lab
- J. Pfaendtner, K. Fleming, "Using Metadynamics for Quantitative Estimates of Chemical Reaction Kinetics," ACS Spring Annual Meeting, 2016, San Diego, CA
- K. Sprenger, T. Weidner, J. Pfaendtner, "Combining Simulation and Spectroscopy to Determine the Structure and Orientation of a Carbohydrate Binding Module (CBM) Inspired Model Peptide on Cellulose," AIChE Annual Meeting, 2016, San Francisco, WA.

- K. Sprenger, S. Summers, J. Kaar, J. Pfaendtner, "Understanding the Structure and Function of Enzymes in ILs for Improved Biocatalysis," poster, AIChE Annual Meeting, 2016, San Francisco, CA.
- K. Sprenger, J. Pfaendtner, "Probing How Defects in Self-Assembled Monolayers Affect Protein Adsorption with Molecular Simulation," AIChE Annual Meeting, 2015, Salt Lake City, UT
- K. Sprenger, J. Pfaendtner, "Probing How Defects in Self-Assembled Monolayers Affect Protein Adsorption with Molecular Simulation," poster, AIChE Annual Meeting, 2015, Salt Lake City, UT
- K. Sprenger, J. Pfaendtner, "Probing How Defects in Self-Assembled Monolayers Affect Protein Adsorption with Molecular Simulation," poster, FOMMS Meeting, 2015, Mt. Hood, OR
- Hough, D. Schwartz, J. Pfaendtner, "Application of a Semi-Detailed Kinetic Model for Lignin Fast Pyrolysis," AIChE Annual Meeting, 2015, Salt Lake City, UT
- K. Oleson, K. Sprenger, J. Pfaendtner, D. Schwartz, "Application of a Semi-Detailed Kinetic Model for Lignin Fast Pyrolysis," AIChE Annual Meeting, 2015, Salt Lake City, UT
- K. Fleming, J. Pfaendtner, "Molecular simulation of hydrolysis reactions to engineer more efficient biomass conversion," American Chemical Society Annual Meeting, Denver, CO, March 23, 2015.
- K. Fleming, J. Pfaendtner, "Probing Reaction Details Critical for Converting Biomass to Fuel Using Molecular Simulation," poster, AAAS National Meeting, San Jose, CA, February 15, 2015.
- J. Pfaendtner, "Molecular Simulation of the Enzymatic Conversion of Biomass in Ionic Liquids," 23rd International Symposium on Chemical Reaction Engineering (ISCRE), 2014, Bangkok Thailand
- V.W. Jaeger, J. Pfaendtner, "Molecular Scale Insights of the Structure Selective Growth of Bionanostructures: A Coarse-Grained and Metadynamics Based Study of Biosilica," poster, AIChE Annual Meeting, 2014, Atlanta, GA
- V.W. Jaeger, J. Pfaendtner, "Understanding the Behavior of Human Serum Albumin in Ionic Liquids Using Molecular Dynamics and Metadynamics," poster, AIChE Annual Meeting, 2014, Atlanta, GA
- K. Fleming, J. Pfaendtner,"Molecular simulation of hydrolysis reactions to engineer more efficient biomass conversion," American Chemical Society Annual Meeting, 2015 Denver, CO
- K. Fleming, J. Pfaendtner, "Probing Reaction Details Critical for Converting Biomass to Fuel Using Molecular Simulation," poster, AAAS National Meeting, 2015, San Jose, CA
- K.G. Sprenger, M. Deighan, J. Pfaendtner, "Elucidating the role of ion concentration and peptide/surface charge on the adsorption thermodynamics of model peptides on self-assembled monolayers, with molecular simulation," AIChE Annual Meeting, 2014, Atlanta, GA.
- K. G. Sprenger, V. Jaeger, J. Pfaendtner, "A Molecular Dynamics Study Assessing the Accuracy of the Generalized Amber Force Field to Predict the Thermophysical Properties of 19 Ionic Liquids," poster, AIChE Annual Meeting, 2014, Atlanta, GA.
- P.R. Burney, N. White, J. Pfaendtner, "Structural Effects of Methionine Oxidation on Isolated Subdomains of Human Fibrin," poster, Biophysical Society Annual Meeting, 2014, San Francisco, CA
- K. Sprenger, J. Pfaendtner, F. Resende, "Conversion of Supercritical Bioethanol into Hydrocarbons over HZSM-5 Zeolite," poster, AIChE Annual Meeting, 2013, San Francisco, CA

- V. Jaeger, P. Burney, J. Pfaendtner, "Comparison of Ionic Liquid-Tolerant Glycoside Hydrolases Using Molecular Dynamics," AIChE Annual Meeting, 2013, San Francisco, CA
- V. Jaeger, J. Pfaendtner, "A Molecular Dynamics Study of the Effects of Ionic Liquids on Human Serum Albumin," poster, AIChE Annual Meeting, 2013, San Francisco, CA
- M. Deighan, T. Weidner, and J. Pfaendtner, "Structural Insights on the N-terminal Binding Domain of Statherin," Biophysical Society Annual Meeting, 2014, San Francisco, CA
- K. Fleming, J. Pfaendtner, "Computational Investigation of Solvent Effects on the Hydrolysis of Ether Linkages," AIChE Annual Meeting, 2013, San Francisco, CA.
- K. Fleming, J. Matthaei, J. Richards, D. Pozzo, J. Pfaendtner, "A New Graduate Level Seminar to Prepare Students for the Next Step in their Careers," poster, AIChE Annual Meeting, 2013, San Francisco, CA.
- J. Pfaendtner, "Molecular Simulation of Biomolecules in Non-Aqueous Media: Application to Lipase and Glycoside Hydrolase," 35th Biotechnology for Fuels & Chemicals Symposium, 2013, Portland, OR
- P. Burney, J. Pfaendtner, "Simulations of *Candida Rugosa* Lipase A in water and nonaqueous solvents," AIChE Annual Meeting, 2012, Pittsburgh, PA
- K. Fleming, J. Pfaendtner, "Enhanced Sampling with Ab Initio Dynamics to Sample Sugar Hydrolysis Reaction Pathways," poster, AIChE Annual Meeting, 2012, Pittsburgh, PA
- K. Fleming, J. Pfaendtner, "Characterization of the Hydrolysis of β-1,4 Glycosidic Bonds," AIChE Annual Meeting, 2012, Pittsburgh, PA
- V. Jaeger, J. Pfaendtner, "Simulations of Biomolecules in Nonaqueous Solvents," poster, AIChE Annual Meeting, 2012, Pittsburgh, PA
- J. Pfaendtner, "Parallel Tempering Metadynamics in the Well Tempered Ensemble: Getting More and Spending Less," AIChE Annual Meeting, 2012, Pittsburgh, PA
- M. Deighan, J. Pfaendtner, "Adsorption of Model Peptides and the Carbohydrate Binding Module: An Enhanced Sampling Molecular Dynamics Study," AIChE Annual Meeting, 2012, Pittsburgh, PA
- V. Jaeger, J. Pfaendtner, "Enzymatic Hydrolysis of Cellulosic Biomass in Nonaqueous Solvents," AIChE Annual Meeting, 2012, Pittsburgh, PA
- J. Pfaendtner, "Using Simulations to Study Biochemistry of Xylanase and Lipase in Ionic Liquids," poster, 2012 German American Frontiers of Science, Potsdam Germany, 2012.
- K. Fleming, J. Pfaendtner, "Quantum Characterization of the Retaining Glycoside Hydrolase Reaction Mechanism for use in Hydrolysis of Xylan," poster, Computational Material Science for Energy Generation and Conversion conference, Santiago, Chile, January 19, 2012.
- J. Pfaendtner, D. Pozzo, "Integration of the Unit Operations Laboratory with a Focus On Biofuel Production," AIChE Annual Meeting, 2011, Minneapolis MN.
- J. Pfaendtner, D. Pozzo, "Integration of the Unit Operations Laboratory with a Focus On Biofuel Production," poster, ASEE Annual Meeting, 2011, Vancouver, BC.
- M. Deighan, J. Pfaendtner,"A Comparative Study on the Enhanced Sampling of Tryptophan-cage Protein," poster, AICHE National Meeting, Minneapolis, Minnesota, 2011.
- P. Burney, J. Pfaendtner," Molecular and Coarse-Grained Analysis of Flap Motion in Lipase Enzymes," poster, AICHE National Meeting, Minneapolis, Minnesota, 2011.

- J. Pfaendtner, “Equilibrium scattering from non-equilibrium MD simulations?,” poster, ORNL ModSim workshop, November 2011, Oak Ridge TN