Jim Pfaendtner

Department of Chemical Engineering
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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
Thesis title: *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

2015—present. Associate Professor of Chemical Engineering, The University of Washington
Since 2016: Jagjeet and Janice Bindra Endowed Career Development Professor
2014-2016: Steven R. and Connie R. Rogel Faculty Fellow
2017—present. Senior Data Science Fellow, University of Washington eScience Institute
2016—present. Senior Scientist, Pacific Northwest National Lab
2013—present. Adjunct Professor of Chemistry, The University of Washington

2009—2015. Assistant Professor of Chemical Engineering, The 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 OpenEye Outstanding Junior Faculty Award
2012. NSF CAREER
2012. Kavli Fellow, US National Academy of Science
2011. ACS PRF Doctoral New Investigator Award
2007. NSF International Research Fellowship

IV. PUBLICATIONS

58. B. Hough, 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", *Comp and Chem Eng*., 2016*, under review*. DOI:

57. C.D. Fu, L.F.L. Oliveira, J. Pfaendtner, "Determining Energy Barriers and Selectivities of a Multi-Pathway System With Infrequent Metadynamics", *J. Chem. Theor. Comput.*, 2016, *in press*. DOI:

56. H. Lutz, V. Jaeger, 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, *in press,* ***DOI:*** *10.1002/psc.2960*

55. V. Jaeger, 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

54. W. A. Beckner, 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

53. H. Tung, 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

52. B. Hough, D. T. Schwartz, J. Pfaendtner, "Detailed kinetic modeling of lignin pyrolysis for process optimization," *IECR*, 2016, 55(34), 9147-9153. DOI: 10.1021/acs.iecr.6b02092

51. R. Pandey, K. Usui, R.A. Livingstone, S.A. Fischer, 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", *Science Advances*, 2016, 2(4), e1501630. DOI: 10.1126/sciadv.1501630

50. K.G. Sprenger, 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, eds Randy Q. Snurr, Claire Adjiman and David Kofke. DOI: 10.1007/978-981-10-1128-3_2

49. K.G. Sprenger, J. Pfaendtner, "Using molecular simulation to study biocatalysis in ionic liquids", *(invited contribution),* in to Methods in Enzymology, 2016, 577, 419-441, ed. Gregory A. Voth. DOI: 10.1016/bs.mie.2016.05.020

48. K.G. Sprenger and 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

47. C. Krumm, J. Pfaendtner, P.J. Dauenhauer, "Millisecond Pulsed Films Unify the Mechanisms of Cellulose Fragmentation", *Chemistry of Materials*, 2016, 28(9), 3108-3114. DOI:10.1021/acs.chemmater.6b00580

46. D. Beck, J.M. Carothers, V. Subramanian, J. Pfaendtner, "Data science: Accelerating innovation and discovery in chemical engineering", *AIChE Journal,* 2016, 62(5), 1402-1416. DOI: 10.1002/aic.15192

45. M. Donovan, Y. Yimmer, J. Pfaendtner, E. Backus, M. Bonn, T. Weidner, "Ultrafast reorientational dynamics of leucine at the air-water interface", *JACS,* 2016, *138* (16), 5226–5229. DOI: 10.1021/jacs.6b01878

44. K.G. Sprenger, A. Choudhury, J. 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

43. K. Fleming, 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]

42. 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

41. J. Pfaendtner, M. Bonomi, "Efficient sampling of high-dimensional free-energy landscapes with Parallel Bias Metadynamics", *J. Chem. Theor. Comput.,* 2015, 11(11), 5062-5067. DOI: 10.1021/acs.jctc.5b00846

40. H. Lutz, V.W. Jaeger, R. Berger, M. Bonn, J. Pfaendtner, T. Weidner, "Biomimetic Growth of Ultrathin Silica Sheets Using Artificial Amphiphilic Peptides", *Advanced Materials Interfaces*, 2015, 2(17), e1500282. DOI: 10.1002/admi.201500282

39. P. de la Iglesia, V.W. Jaeger, 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

38. Z. Levine, S.A. Fischer, J.E. Shea and J. Pfaendtner, "Trp-Cage Folding on Organic Surfaces", *J. Phys. Chem. B.*, 2015, 119(3), 10417-10425. DOI: 10.1021/acs.jpcb.5b04213

37. 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

36. K. G. Sprenger, V.W. Jaeger, 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

35. P. Burney, E. M. Norwald, K. Hickman, 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

34. G. Newbloom, S. Hoffmann, A. West, M. Gile, 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

33. V. Jaeger, P. Burney, J. Pfaendtner, "Comparison of Three Ionic Liquid Tolerant Cellulases by Molecular Dynamics", *Biophysical Journal,* 2015, 108(4), 880-892. DOI: 10.1016/j.bpj.2014.12.043

32. K. Fleming, J. Matthei, J. Pfaendtner, "A new graduate level seminar to prepare students for the next step in their career", *Chemical Engineering Education,* 2015, 49(1) 29-37.

31. S. Zheng, J. Pfaendtner, "Enhanced sampling of chemical and biochemical reactions with metadynamics", *Molecular Simulation,* 2015, 41(1-3), 55-72. DOI: 10.1080/08927022.2014.923574 [invited review]

30. J. E. Baio, A. Zane, V. Jaeger, A.M. Roehrich, H. Lutz, J. Pfaendtner, G P. Drobny, and T Weidner, "Diatom mimics: directing the formation of biosilica nano-particles by controlled folding of lysine-leucine peptides", *JACS,* 2014, 136(43), 15134-15137. DOI: 10.1021/ja5078238

29. S. Zheng, 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. DOI: 10.1021/jp500398k

28. Z. Jarin and J. Pfaendtner, "Ionic Liquids Can Selectively Change the Conformational Free-Energy Landscape of Sugar Rings", *J. Chem. Theor. Comput.*, 2014, 10(2), 507-510. DOI: 10.1021/ct4010036

27. P. Burney, 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.

26. A. Paulson, B. Hough, 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)", *Chem Sus Chem,* 2014, 7(3), 765-776

25. A. Barducci, A. J. Pfaendtner, J., M. Bonomi, "Tackling Sampling Challenges in Biomolecular Simulations", In *Molecular Modeling of Proteins*, Kukol, A., Ed. Springer New York: New York, NY, 2015; pp 151-171.

24. 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.

23. M. Deighan, J. Pfaendtner, "Exhaustively Sampling Peptide Adsorption with Metadynamics", *Langmuir,* 2013, 29(25), 7999-8009. DOI: 10.1021/la4010664

22. A. White, A. Keefe, J. R. Ella-Menye, A. Nowinski, Q. Shao, J. Pfaendtner, S. Jiang, "Insights into Solvated Salt Bridges", *J. Phys. Chem. B,* 2013, 117(24), 7254-7259.

21. V. Jaeger and J. Pfaendtner, "Structure, Dynamics and Activity of Xylanase Solvated in Binary Mixtures of Ionic Liquid and Water", *ACS Chemical Biology,* 2013, 117(9), 2662-2670. DOI: 10.1021/cb3006837

20. P. Burney and J. Pfaendtner, "Structural and dynamic features of *Candida rugosa* Lipase1 in Water, Octane, Toluene, and Ionic Liquids BMIM-PF6 and BMIM-NO3", *J. Phys. Chem. B*, 2013, 117, 2662-2670.

19. M. Deighan, M. Bonomi, J. Pfaendtner, "Efficient Simulation of Explicitly Solvated Proteins in the Well-Tempered Ensemble", *J. Chem. Theor. Comp.*, 2012, 8, 2189-2192. DOI: 10.1021/ct300297t

18. 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.

17. J. Pfaendtner, E. M. De La Cruz, and G. A. Voth, "Actin Filament Remodeling by Cofilin," *Proc. Natl. Acad. Sci. USA*, 2010, 97 *(16)*, 7299-7304.

16. J. Pfaendtner, D. Branduardi, M. Parrinello, T. D. Pollard, and G. A. Voth, "Nucleotide-Dependent

Conformational States of Actin," *Proc. Natl. Acad. Sci. USA,* 2009, *106* (31), 12723-12728.

15. J. Pfaendtner., E. Lyman, T. D. Pollard, and G. A. Voth., "Structure and dynamics of the actin filament," J. *Mol. Biol.*, 2010, 396 *(2)*, 252-263. [*selected for cover article*]

14. Zhang, Z., J. Pfaendtner, A. Grafmüller, and G. A. Voth, "Defining coarse-grained representations of large biomolecules and biomolecular complexes from elastic network models," *Biophys. J.*, 2009, 97 *(8)*, 2327-2333.

13. 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.

12. J. Pfaendtner and G. A. Voth, "Molecular Dynamics Simulation and Coarse-grained Analysis of the Unactivated Arp2/3 Complex," *Biophys. J.,* 2008, *95* (11), 5324-5333.

11. E. Lyman, J. Pfaendtner, G. A. Voth, "Systematic Multiscale Parameterization of Heterogeneous Elastic Network Models of Proteins*," Biophys. J.,* 2008, *95* (9), 4183-4192.

10. Z. Zhang, L. Lu, W. G. Noid, V. Krishna, J. Pfaendtner, G. A. Voth, "A Systematic Methodology for Defining Coarse-grained Sites in Large Biomolecules," *Biophys. J.*, 2008, 95 *(11)*, 5073-5083.

9. X. Yu, J. Pfaendtner, and L. J. Broadbelt, "Ab Initio Study of Acrylate Polymerization Reactions: Methyl Methacrylate and Methyl Acrylate Propagation*," J. Phys. Chem. A*, 2008, *112* (29), 6772-6782.

8. J. Pfaendtner and L. J. Broadbelt, "Mechanistic Modeling of Lubricant Degradation Part 1: Structure-Reactivity Relationships for Free-Radical Oxidation," *Ind. Eng. Chem. Res.*, 2008, *47* (9), 2886-2896.

7. J. Pfaendtner and L. J. Broadbelt, "Mechanistic Modeling of Lubricant Degradation Part 2: The Autoxidation of Octane and Decane*," Ind. Eng. Chem. Res.*, 2008, *47* (9), 2897-2904.

6. M. Siniawski, N. Saniei, and J. Pfaendtner, "Tribological Degradation of Two Vegetable-Based Lubricants at Elevated Temperatures," *J. Synth. Lubr.*, 2007, *24* (3), 167-169.

5. J. Pfaendtner and 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, and L. J. Broadbelt, "The 1D Hindered Rotor Approximation," *Theor. Chem. Acc.*, 2007, *118* (5-6), 881-898.

3. J. Pfaendtner and 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, and 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 and J. Pfaendtner, "Lexicography of Kinetic Modeling of Complex Reaction Networks*," AIChE. J.*, 2005, *51* (8), 2112-2121.

V. TEACHING

V-I. INDIVUDAL INSTRUCTION

Former Postdoctoral or Graduate Advisees

Dr. Yeneneh Yimer [postdoc 2014-2106]
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
Wesley Beckner
Garrett Davidson
Luke Gibson
Christopher Fu
Moke Mao
Tai-Yu Pan
Arushi Prakash (co-advised with Christopher J. Mundy, PNNL)
Kushmeen Sakloth
Joshua Smith (co-advised with Shaoyi Jiang)
Kayla Sprenger
Kejia Wu

Former and Current Undergraduate Researchers and REU students

Melissa Gile, Peter Englund, Christopher Fu, Nikita Grover, Katie Hoffman, Samuel Hwang, Miwakoto 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

	Course	Year/Quarter Taught	Instructor Ranking[1]	
			"Instructor's effectiveness in teaching the course"	"Instructor's contribution to the course"
University of Washington	CHEM E 435 (*mass transfer and separations)*	F14	4.8 (5.0)	4.7 (4.9)

		F15	4.6 (4.9)	4.8 (5.1)
		F16	3.4 (3.8)	3.7 (4.1)
	CHEM E 465	F10	4.6 (4.8)	4.8 (5.0)
	(*reactor design)*	F11	4.7 (5.1)	4.6 (4.9)
		F12	4.8 (5.2)	4.9 (5.3)
		F13	4.9 (5.1)	4.8 (5.0)
	CHEM E 375	W10	4.5 (4.2)	4.5 (4.3)
	(computer skills)	W11	4.7 (4.5)	4.9 (4.7)
		W12	4.9 (4.5)	4.9 (4.5)
		W13	4.8 (4.6)	4.7 (4.5)
		W14	4.9 (4.7)	4.9 (4.7)
		W15	4.9 (4.6)	4.9 (4.6)
		W16	4.8 (4.4)	4.8 (4.4)
	CHEM E 437[2]	W11	4.7 (4.5)	4.5 (4.4)
	(senior lab)	W12	3.6 (3.9)	3.7 (3.9)
	CHEM E 485	W13	4.9 (5.0)	4.8 (5.2)
	(senior design I)	W14	4.9 (4.9)	4.7 (4.8)
	CHEM E 599	SP10	4.8 (4.7)	4.5 (4.3)
	(multiscale modeling)			

[1]Unless noted the scale of rankings is from 0-5. UW adjusts mean values based on certain course criteria such as difficulty, the adjusted means are also provided 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

1) Departmental and University Contributions

- COE Ad Hoc Committee on leadership development, 2016-17
- UW Provost Leadership Excellent Program, 2015-2017
- UW Husky 100 Advisory Board, 2016-17
- Center for Teaching and Learning "Senior Fellow", 2016-17
- 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 and Safety" Faculty Advisory Committee to UW President, 2015-2017
- Graduate Program Director, 2014 – present
- 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
- Department Faculty Search Committee, 2011-2014 [search co-chair 2013-14]
- Civil and Environmental Engineering Search Committee 2013-2014
- Department Computer Committee, 2009-present
- 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-present
- Faculty Advisor for Tau Beta Pi (Undergrad Engineering Honor Society), 2012-present
- Faculty Advisor for ACES (Graduate Student Professional Organization), 2009-2012 , 2014-present
- Organizer of Department Seminar Series, 2009-2012
- Guest lecture in 6 Molecular and Engineering Science seminar/classes ranging from undergraduate to graduate level, 2009-2015
- Panelist at UW ADVANCE CAREER workshop, 2012, 2014
- Panelist at UW NSF GRF workshop, 2012-15
- 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

2) 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)

3) Scientific Reviews and Panels

2016: Reviewer for 1 NSF panel, ad hoc review for Belgium Science Foundation 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

4) Journal Referee and Editorial

Journal Referee for ACS Catalysis, AIChE Journal, Applied Catalysis B: Environmental, Applied Physics A, Biochemistry, BioEnergy Research, Biophysical Journal, Biotechnology and 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, JACS, Journal of Chemical Information and Modeling, Journal of Molecular Graphics and 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

5) Industrial/Corporate

- 2010 – 2014: Consulting in research on kinetics of food chemistry for a Fortune 500 company specializing in food and beverage (~30 days/year)

VII. RESEARCH FUNDING AS PI OR CO-PI SINCE 2007 [TOTAL ~ $8.3 MILLION]

1. NSF International Research Fellows Program [9/1/07 – 8/31/09]
    a. Project Title: Biomass-Derived Fuels: Modeling and Simulation of Enzymatic Processes
    b. Funding: $156,000
2. NSF BRIGE Program [9/1/10 – 8/31/13]
    a. Project Title: Understanding Protein-Surface Interactions Through Multiscale Modeling: Application to Biofuel Cells
    b. Funding: $187,172
3. NSF CCLI (Lab / Education Grant) [PI: L.D. Pozzo, UW]
    a. Co-PI: Jim Pfaendtner
    b. Project Title: A Consolidated Chemical Engineering Laboratory with a Focus on Bioenergy
    c. Funding: $199,360
4. NSF EAGER [1/15/11 – 1/14/12]
    a. Project Title: COLLABORATIVE RESEARCH: Pyrolysis of Cellulose Intermediate Liquids: Automated Mechanism Development and Experimental Characterization
    b. Co-PI: Paul Dauenhauer, UMASS
    c. Funding: $79,999 (total)
5. NSF Pan American Advanced Studies Institute [12/1/11 – 11/30/12]
    a. Co-PI: Cameron Abrams, Drexel
    b. Project Title: Molecular-Based Multiscale Modeling and Simulation; Montevideo, Uruguay; September 1-14, 2012
    c. Funding: $100,000
6. NSF CAREER [3/15/12 – 3/14/17]
    a. Project Title: Computational Enzymology of Non-Aqueous Biocatalysis – Application to Biomass Pretreatment
    b. Funding: $484,750
7. NSF Catalyzing New International Collaborations [5/1/12 – 4/30/13]
    a. Project Title: Integrating Multiscale Modeling With Protein-Surface Experiments
    b. Funding: $17,262
8. AFOSR Core Funding [4/1/12 – 3/31/15]
    a. Project Title: Automated Discovery of Energetic Ionic Liquid Chemistry: Reaction Topology, Thermochemistry and Kinetics
    b. Funding: $360,000
9. ACS PRF Doctoral New Investigator Program [9/1/2012 – 8/31/14]
    a. Project Title: Theoretical Considerations of Conjugated Polymer Self-Assembly
    b. Funding: $100,000
10. NSF CBET Core Funding [8/1/13 – 7/30/16]

   a. Project Title: NSF-DFG: Combining Simulation and Spectroscopy to Determine the Structure and Dynamics of Adsorbed Proteins - Application to Biomass Conversion
      i. Exploratory international collaboration program between NSF and German DFG initiated by J. Pfaendtner. JP received funding from the NSF and a separate proposal was reviewed by the DFG for funding Dr. Tobias Weidner
   b. Funding: $308,000
11. Exploratory research project with Boeing corporation [8/1/13 – 12/31/15]
   a. Project Title: Feasibility study for a novel high throughput virtual screening of adhesive/coating compounds
   b. Funding: $241,000
12. UW RRF (internal seed project funding) [9/1/14 – 8/31/15]
   a. Project Title: Multiscale Modeling Investigation of Peptide Self-Assembly in the Formation of Nanostructures
   b. Funding: $34,932
13. UW STF (student tech fee grant program) [7/1/15 – 6/30/20]
   a. Project Title: High Performance Computing for All Students
   b. Funding: ~$800,000
14. AFOSR Core Funding [~10/1/15 – 9/30/18]
   a. Project Title: Interrogating Dynamic, Stochastic and Topological Features of Reaction Networks: Application to Combustion Chemistry
   b. Funding: $510,000
15. Co-PI on NSF NNCI: Northwest Nanotechnology Infrastructure (NWNI)
   a. JP role: co-PI and lead of computational/modeling thrust for large instrumentation / shared infrastructure grant
   b. Funding: $4,500,000 (JP portion: $0)
16. Co-PI on NSF MRI Program Grant [9/1/2016 – 8/31/2019]
   a. Project Title: MRI: Acquisition of a Shared Next-Generation Computer Cluster to Advance Molecular to Nanoscale Science and Engineering
   b. JP role: co-PI
   c. Funding: $622,000
17. PI on NSF NRT Training Grant [9/1/2016 – 8/31/2021]
   a. Project Title: NRT-DESE: Data Intensive Research Enabling Clean Technologies (DIRECT)
   b. JP role: PI and director
   c. Funding: ~3,800,000
18. PI on UW Clean Energy Institute Faculty Exploration Grant [9/15/2016 – 6/15/2017]
   a. Project Title: Predictive modeling to integrate the physics of battery electrolyte materials with the performance of renewable energy grids
   b. JP role: PI
   c. Funding: $36,124
19. PNNL Subcontract [6/15/2015 – 12/31/2018]
   a. Project Title: Modeling and Simulation of Peptoids
   b. JP role: PI
   c. Total funding expected during project period: ~$300,000

VIII. PRESENTATIONS

VIII-I. INVITED PRESENTATIONS (SINCE 2009)

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", presented at the AIChE Annual Meeting, 2016, San Francisco, CA

J. Pfaendtner, "Using Molecular Dynamics to Study Complex Reacting Systems", presented at Telluride Science Research Center Workshop on Complex Reacting Systems, 2016

J. Pfaendtner, "Advanced Methods in Enhanced Sampling", Presented at 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 ", presented at the 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 and Biological Engineering seminar, 2015

J. Pfaendtner, "Using computer simulations to engineer new solvents and interfaces for controlling the behavior of biomolecules", Zhejiang University Chemical and 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 seminar, 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 and 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", presented at the 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", UC Santa Barbara BMSD seminar, 2013

J. Pfaendtner, "Enhanced Sampling of Peptide Adsorption and 2D Self-Assembly with Parallel

Tempering Metadynamics", presented at the AIChE Annual Meeting, 2012, Pittsburgh, PA

J. Pfaendtner, "Applications of "Bottom Up" Multiscale Modeling: Uncovering the Role of Solvents and Surfaces", USC 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?", UW Materials Science and 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?", Presentation at 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", UW Physical Chemistry Seminar Series, 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", UW Center for Nanotechnology, 2010.

J. Pfaendtner, "The Origin Of Nucleotide-Dependent Properties In The Actin Filament: A Multiscale Study", presented at Third International Conference on Mechanics of Biomaterials & Tissues, Clearwater Beach, 2009.

J. Pfaendtner, "Simulation Reveals Fundamental Behavior of the Actin Filament and Arp2/3 Branch Junction", presented at the CECAM workshop on Coarse-Graining Biological Systems: Towards Large-Scale Interactions and Assembly, Lausanne, Switzerland, 2009.

J. Pfaendtner, "Multiscale Modeling of Actin: Nucleotide-Dependent Properties and the Arp2/3 Branch Junction", MIT Chemical Engineering Seminar, 2009.

J. Pfaendtner, "Multiscale Modeling of Actin: Nucleotide-Dependent Properties and the Arp2/3 Branch Junction", University of Washington Chemical Engineering Seminar, 2009.

J. Pfaendtner, "Multiscale Modeling of Actin: Nucleotide-Dependent Properties and the Arp2/3 Branch Junction", Rice University Chemical Engineering Seminar, 2009.

J. Pfaendtner, "Multiscale Modeling of Actin: Nucleotide-Dependent Properties and the Arp2/3 Branch Junction", Carnegie Mellon Chemical Engineering Seminar, 2009.

VIII-II. CONTRIBUTED PRESENTATIONS (SINCE 2009)

J. Pfaendtner, "Quantitative Estimates of Chemical Kinetics With Metadynamics", MACCCR Meeting, 2016, Argonne National Lab

J. Pfaendtner, Kelly Fleming, "Using Metadynamics for Quantitative Estimates of Chemical Reaction Kinetics", ACS Spring Annual Meeting, 2016, San Diego, CA

K. Sprenger, J. Pfaendtner, "Probing How Defects in Self-Assembled Monolayers Affect Protein Adsorption with Molecular Simulation," presentation at the 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 presentation at the 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 presentation at FOMMS Meeting, 2015, Mt. Hood, OR

B. Hough, D. Schwartz, J. Pfaendtner, "Application of a Semi-Detailed Kinetic Model for Lignin Fast Pyrolysis," presentation at the 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," presentation at the AIChE Annual Meeting, 2015, Salt Lake City, UT

K. Fleming, J. Pfaendtner, "Molecular simulation of hydrolysis reactions to engineer more efficient biomass conversion," presentation at the 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 Presentation at the AAAS National Meeting, San Jose, CA, February 15, 2015.

J. Pfaendtner, "Molecular Simulation of the Enzymatic Conversion of Biomass in Ionic Liquids", presented at the 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 presented at the 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 presented at the AIChE Annual Meeting, 2014, Atlanta, GA

K. Fleming, J. Pfaendtner, "Molecular simulation of hydrolysis reactions to engineer more efficient biomass conversion," presented at the 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 presented at the 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", presented at the 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 presented at the 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 presented at the 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 presented at the AIChE Annual Meeting, 2013, San Francisco, CA

V. Jaeger, P. Burney, J. Pfaendtner, "Comparison of Ionic Liquid-Tolerant Glycoside Hydrolases Using Molecular Dynamics", presented at the 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 presented at the AIChE Annual Meeting, 2013, San Francisco, CA

M. Deighan, T. Weidner, and J. Pfaendtner, "Structural Insights on the N-terminal Binding Domain of Statherin", presented at the 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 presented at the AIChE Annual Meeting, 2013, San Francisco, CA.

J. Pfaendtner, "Molecular Simulation of Biomolecules in Non-Aqueous Media: Application to Lipase and Glycoside Hydrolase", presented at the 35th Symposium on Biotechnology for Fuels and Chemicals, 2013, Portland, OR

P. Burney, J. Pfaendtner, "Simulations of *Candida Rugosa* Lipase A in water and nonaqueous solvents", presented at the AIChE Annual Meeting, 2012, Pittsburgh, PA

K. Fleming, J. Pfaendtner, "Enhanced Sampling with Ab Initio Dynamics to Sample Sugar Hydrolysis Reaction Pathways", poster presented at the AIChE Annual Meeting, 2012, Pittsburgh, PA

K. Fleming, J. Pfaendtner, "Characterization of the Hydrolysis of β-1,4 Glycosidic Bonds", presented at the AIChE Annual Meeting, 2012, Pittsburgh, PA

V. Jaeger, J. Pfaendtner, "Simulations of Biomolecules in Nonaqueous Solvents", poster presented at the

AIChE Annual Meeting, 2012, Pittsburgh, PA

J. Pfaendtner, "Parallel Tempering Metadynamics in the Well Tempered Ensemble: Getting More and Spending Less", presented at the 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", presented at the AIChE Annual Meeting, 2012, Pittsburgh, PA

V. Jaeger, J. Pfaendtner, "Enzymatic Hydrolysis of Cellulosic Biomass in Nonaqueous Solvents", presented at the AIChE Annual Meeting, 2012, Pittsburgh, PA

J. Pfaendtner, "Using Simulations to Study Biochemistry of Xylanase and Lipase in Ionic Liquids", poster presentation at the 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 presentation at the 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 presented at the ASEE Annual Meeting, 2011, Vancouver, BC.

M. Deighan, J. Pfaendtner, "A Comparative Study on the Enhanced Sampling of Tryptophan-cage Protein", poster presented at AICHE National Meeting, Minneapolis, Minnesota, 2011.

P. Burney, J. Pfaendtner, " Molecular and Coarse-Grained Analysis of Flap Motion In Lipase Enzymes", poster presented at AICHE National Meeting, Minneapolis, Minnesota, 2011.

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