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Personal

Date of birth:	27 February 1972
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Spouse:	Lisa J. Lobree, Ph.D.
Children:	Emma K. (b. 2002), Stella G. (b. 2004), and Samuel C. (b. 2007)

Degrees

North Carolina State University, B.S. Chemical Engineering (*summa cum laude*), 1995
University of California, Berkeley, Ph.D. Chemical Engineering, 2000
Thesis: *Molecular Dynamics Simulations of Plasma-Surface Chemistry*
Advisors: Profs. David Graves (chair), Arup Chakraborty, Martin Head-Gordon

Professional Experience

Drexel University, Department of Chemical and Biological Engineering

Department Head	2017-
Professor	2012-
Associate Professor	2008-2012
Assistant Professor	2002-2008

Drexel University College of Medicine, Department of Biochemistry and Molecular Biology

Professor	2012-

Max-Planck-Institute for Polymer Research, Mainz, Germany

Postdoc, Theory Group	2000-2002

University of California, Berkeley, Department of Chemical Engineering

Graduate Research Assistant	1995-2000
Graduate Teaching Assistant	1995-1997

North Carolina State University, Raleigh, North Carolina, Department of Chemical Engineering and Department of Computer Science

Undergraduate Teaching Assistant	1993-1995

Eastman Chemical, Columbia, South Carolina

Summer Intern	1994

Dupont, Dacron Technical Research Lab, Kinston, North Carolina

Co-op Engineer	1991-1993

Publications

110. Melissa Grenier, Shilei Ding, Dani Vézina, Jean-Philippe Chapleau, William Tolbert, Rebekah Sherburn, Arne Schon, Sambasivarao Somisetti, Cameron F. Abrams, Marzena Pazgier, Andrés Finzi, and Amos B. Smith III "Optimization of Small Molecules for their Capacity to Sensitize HIV-1 Infected Cells to Antibody Dependent Cellular Cytotoxicity," *ACS Med. Chem. Lett.* (accepted, 2019) (10.1021/acsmedchemlett.9b00445)
109. Jasmine Gardner and Cameron F. Abrams, "Energetics of Flap Opening in HIV-1 Protease: String Method Calculations," *J. Phys. Chem. B* **123**:9584-9591 (2019) (10.1021/acs.jpcb.9b08348)

108. Anindya Bhaduri, Jasmine Gardner, Cameron F. Abrams, and Lori Brady, "Free energy calculation using space filled design and weighted reconstruction: A modified single sweep approach," *Mol. Sim.* (accepted, 2019) (10.1080/08927022.2019.1688325)
107. Shilei Ding, Melissa Grenier, William Tolbert, Dani Vézina, Rebekah Sherburn, Jonathan Richard, Jérémie Prévost, Jean-Philippe Chapleau, Gabrielle Gendron-Lepage, Halima Medjahed, Cameron Abrams, Joseph Sodroski, Marzena Pazgier, Amos Smith III, and Andrés Finzi , "A new family of small-molecule CD4-mimetic compounds contact the highly conserved aspartic acid 368 of HIV-1 gp120 and mediates ADCC," *J. Virol.* **93:**e01325-19 (2019) (10.1128/JVI.01325-19)
106. Gourav Shrivastav, Eric Vanden-Eijnden and Cameron F. Abrams, "Mapping Saddles and Minima on Free Energy Surfaces using Multiple Climbing Strings", *J. Chem. Phys.* **151**:124112 (2019) (10.1063/1.5120372).
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104. Ming Huang and Cameron F. Abrams, "Effects of Reactivity Ratios on Network Topology and Thermomechanical Properties in Vinyl-Ester/Styrene Thermosets: Molecular Dynamics Simulations," *Macromol. Theory. Sim.* **28**:1900030 (2019) (10.1002/mats.201900030).
103. Arun Srikanth Sridhar and Cameron F. Abrams, "Effect of molecular packing and hydrogen bonding on the properties of epoxy-amido amine systems", *Comput. Mater. Sci.* **169**:109082 (2019) (10.1016/j.commatsci.2019.109082).
102. Maolin Lu, Xiaochu Ma, Luis R. Castillo-Menendez, Jason Gorman, Nirmin Alsahafi, Utz Erme, Daniel S. Terry, Michael Chambers, Dongjun Peng, Baoshan Zhang, Tongqing Zhou, Nick Reichard, Kevin Wang, Jonathan Grover, Brennan P. Carman, Matthew R. Gardner, Ivana Nikić-Spiegel, Akihiro Sugawara, James Arthos, Edward A. Lemke, Amos B. Smith III, Michael Farzan, Cameron Abrams, James B. Munro, Adrian B. McDermott, Andrés Finzi, Peter D. Kwong, Scott C. Blanchard, Joseph G. Sodroski and Walther Mothes, "Associating HIV-1 envelope glycoprotein structures with states on virus observed by smFRET", *Nature,* **568**:415-419 (2019) (10.1038/s41586-019-1101-y).
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98. Steven Gossert, Bibek Parajuli, Irwin Chaiken, and Cameron F. Abrams, "Roles of Conserved Tryptophans in Trimerization of HIV-1 Membrane-Proximal External Regions: Implications for Virucidal Design via Alchemical Free-Energy Molecular Simulations," *Proteins,* **86**:707–711 (2018) (10.1002/prot.25504) (PMCID: PMC6013385).
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molecular simulation and experimental study," *Polymer* **90**:249-255 (2016) (10.1016/j.polymer.2016.03.023).
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67. Ali Emileh, Caitlin Duffy, Andrew Holmes, Arangassery Rosemary Bastian, Rachna Aneja, Ferit Tuzer, Srivats Rajagopal, Huiyan Li, Cameron F. Abrams, and Irwin Chaiken, "Covalent conjugation of a peptide triazole to HIV-1 gp120 enables intramolecular binding site occupancy," *Biochemistry* **53**:3402-3414 (2014) (10.1021/bi500136f).
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65. Michelle K. Baker, Vamshi Gangupomu, and Cameron F. Abrams, "Characterization of the water defect at the HIV-1 gp41 membrane spanning domain in bilayers with and without cholesterol using molecular simulations," *BBA-Biomembranes* **1838**:1396-1405 (2014) (10.1016/j.bbamem.2014.01.009).
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63. Mark Contarino, Arangassery R. Bastian, Ramalingam Venkat Kalyana Sundaram, Karyn McFadden, Caitlin Duffy, Vamshi Gangupomu, Michelle Baker, Cameron Abrams, and Irwin Chaiken, "Chimeric Cyanovirin-MPER Recombinantly Engineered Proteins Cause Cell-Free Virolysis of HIV-1," *Antimicrob. Agents Ch.* **57**:4743-4750 (2013) (10.1128/AAC.00309-13).

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60. Ali Emileh, Ferit Tuzer, Herman Yeh, Muddegowda Umashankara, Diogo Moreira, Judith LaLonde, Carole Bewley, Cameron F. Abrams, and Irwin Chaiken, "A Model of the Peptide Triazole Entry Inhibitor Binding to HIV-1 gp120 and Mechanism of Bridging Sheet Disruption," *Biochemistry* **52**:2245–2261 (2013) (10.1021/bi400166b).
59. Mauro Lapelosa and Cameron F. Abrams, "A computational study of water and CO migration sites and channels inside myoglobin," *J. Chem. Theory Comput.* **9**:1265-1271 (2013) (10.1021/ct300862j).
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18. Cameron F. Abrams and Kurt Kremer, "Combined coarse-grained and atomistic simulation of liquid bisphenol-A-polycarbonate: Liquid packing and intramolecular structure," *Macromolecules* **36**:260-267 (2003) (10.1021/ma0213495).

Prior to joining Drexel

17. Luigi Delle Site, Cameron F. Abrams, Ali Alavi, and Kurt Kremer. "Polymers near metal surfaces: Selective adsorption and global conformations," *Phys. Rev. Lett.* **89**:156103 (2002) (10.1103/PhysRevLett.89.156103).
16. Cameron F. Abrams, Namkyung Lee, and Sergei Obukhov. "Collapse dynamics of a homopolymer: Theory and simulation," *Europhys. Lett.* **59**:391-397 (2002) (10.1209/epl/i2002-00207-5).
15. Cameron F. Abrams and Kurt Kremer. "Effects of excluded volume and bond length on the dynamics of dense bead-spring polymer melts," *J. Chem. Phys.* **116**:3162-3165 (2002) (10.1063/1.1445107).
14. Cameron F. Abrams, Luigi Delle Site, and Kurt Kremer, "Multiscale Computer Simulations for Polymeric Materials in Bulk and near Surfaces," in "Bridging Time Scales: Molecular Simulations for the Next Decade," P. Nielaba, M. Mareschal, and G. Ciccotti, eds., *Lecture Notes in Physics* **605**:143 Springer (2002).
13. Cameron F. Abrams and Kurt Kremer. "The effect of bond length on the structure of dense bead-spring polymer melts," *J. Chem. Phys.* **115**:2776-2785 (2001) (10.1063/1.1385791).

Prior to joining MPIP

12. Cameron F. Abrams and David B. Graves. "Atomistic simulation of fluorocarbon deposition on Si by continuous bombardment with energetic CF^+ and CF_2^+," *J. Vac. Sci. Technol. A* **19**:175-181 (2001) (10.1116/1.1322652).
11. Cameron F. Abrams and David B. Graves. "Atomistic simulation of Si etching by energetic CF_3^+: Product distributions and energies," *Thin Solid Films* **374**:150-156 (2000).
10. Cameron F. Abrams and David B. Graves. "Molecular dynamics simulations of Si etching with energetic F^+: Sensitivity of results to the interatomic potential," *J. Appl. Phys.* **88**:3734-3738 (2000) (10.1063/1.1288701).
9. Junichi Tanaka, Cameron F. Abrams and David B. Graves. "New C-F interatomic potential for molecular dynamic simulation of fluorocarbon film formation," *J. Vac. Sci. Technol. A* **18**:938-945 (2000) (10.1116/1.582279).
8. Cameron F. Abrams and David B. Graves. "On the active surface layer in CF_3^+ etching of Si: Atomistic simulation and a simple mass balance model," *J. Vac. Sci. Technol. A* **18**:411-416 (2000) (10.1116/1.582202).
7. Cameron F. Abrams and David B. Graves. "Molecular dynamics simulations of Si etching by energetic CF_3^+ ions," *J. Appl. Phys.* **86**:5938-5948 (1999) (10.1063/1.371637).

6. Cameron F. Abrams and David B. Graves. "Three-dimensional spatiokinetic distributions of sputtered and scattered products of Ar^+ and Cu^+ impacts onto the Cu surface: Molecular dynamics simulations," *IEEE Trans. Plas. Sci.* **27**:1426-1432 (1999) (10.1109/27.799821).
5. Michael A. Vyvoda, Cameron F. Abrams and David B. Graves. "Feature evolution simulation of copper seed layer deposition: Using atomic level particle scattering information," *IEEE Trans. Plas. Sci.* **27**:1433-1440 (1999) (10.1109/27.799822).
4. Cameron F. Abrams and David B. Graves. "Cu^+ bombardment of Cu surfaces at near-threshold energies: Molecular dynamics simulations," *J. Appl. Phys.* **86**:2263-2267 (1999).
3. Cameron F. Abrams and David B. Graves. "Energetic ion bombardment of SiO_2 surfaces: Molecular dynamics simulations," *J. Vac. Sci. Technol. A* **16**:3006-3019 (1998) (10.1116/1.581452).

Prior to attending UC Berkeley

2. W. S. Ahn, Yaping Zhong, Cameron F. Abrams, P. K. Lim, and P. A. Brown. "Biphasic autoxidation of tetralin catalyzed by surface-active transition metal complexes," *J. Phys. Chem. B* **101**:596-602 (1997) (10.1021/jp9627234).
1. Yaping Zhong, Cameron F. Abrams, and P. K. Lim. "Biphasic synthesis of poly(2,6-dimethyl-1,4-phenylene oxide) using a surface-active coupling catalyst. 2. Process improvements, additional kinetic results, and proposed reaction mechanism," *Ind. Eng. Chem. Res.* **34**:1529-1535 (1995) (10.1021/ie00044a003).

Seminars and Presentations

Invited

60. "Recent simulation methods for resolving molecular details in thermodynamics and kinetics," University at Buffalo, Dept. of Chemical and Biological Engineering, 23 October 2019.
59. "Recent simulation methods for resolving molecular details in thermodynamics and kinetics," University of California, Davis, Dept. of Chemical Engineering, 10 October 2019.
58. "Recent simulation methods for resolving molecular details in thermodynamics and kinetics," University of Rhode Island, Dept. of Chemical Engineering, 18 October 2018.
57. "On-the-fly free-energy parameterization: Better statistics in biomolecular simulations from enhanced sampling," Simons Foundation, New York, New York, 13 November 2017.
56. "New Rare-Event Methods in Molecular Simulations: Some Recent Progress", Bristol-Myers-Squibb, New Brunswick, New Jersey, 15 October 2017.
55. "New Rare-Event Methods in Molecular Simulations: Applications to Ligand Entry Kinetics and Protein Conformational Changes", University of New Hampshire, Department of Chemical Engineering, Durham, New Hampshire, 9 September 2017.
54. "Rare-Event Methods in Molecular Simulations: Some Recent Progress", ExxonMobil Central Research and Engineering, Clinton, New Jersey, 4 August 2017.
53. "Thermodynamics and kinetics of biomolecular interactions using molecular simulations", Department of Bioengineering, University of Maryland, College Park, Maryland, 17 March 2017.
52. "Thermodynamics and kinetics of biomolecular interactions using molecular simulations", Department of Chemical and Biomolecular Engineering, University of Pennsylvania, Philadelphia, Pennsylvania, 1 March 2017.
51. "Determining protein conformational statistics using molecular dynamics simulations", Department of Biochemistry and Molecular Biology, Thomas Jefferson University, Philadelphia, Pennsylvania, 31 October 2016.
50. "Recent Advances in Molecular Simulations of Complex Materials and Biomolecules," ExxonMobil Research and Engineering, Paulsboro Technical Center, Paulsboro, New Jersey, 25 October 2016.
49. "Determining conformational statistics of proteins via replica-exchange on-the-fly free-energy parameterization," 252nd National Meeting of the American Chemical Society, Philadelphia, Pennsylvania, 25 August 2016.

48. "The Roles of Intrinsic Curvature and Lipid Sorting on the Stability of Hemifusions via Coarse-Grained Molecular Simulations," CECAM International Workshop on Biomembranes: The Consequences of Complexity, Helsinki, Finland, 16-19 August 2016.
47. "New rare-event methods in molecular simulations: Applications to ligand entry kinetics and protein conformational changes," Center for Biophysics and Computational Biology Seminar, Temple University, 27 April 2016.
46. "New rare-event methods in molecular simulations: Applications to ligand entry kinetics and protein conformational changes," AMCS/PICS Colloquium, The University of Pennsylvania, 15 April 2016.
45. "Markovian Milestoning MD Simulations for Computing On- and Off-Rates," 251st National Meeting of the American Chemical Society, San Diego, California, 12 March 2016.
44. "Markovian Milestoning MD Simulations for Computing On- and Off-Rates," Mathematical Challenges in Protein and Drug Design, Molecular Biosciences Institute, The Ohio State University, Columbus, Ohio, 7-11 December 15.
43. "Small-Molecule Entry and Exit Kinetics in Proteins Computed Using Markovian Milestoning," Plenary Session, Computational Molecular Science and Engineering Forum (CoMSEF), Annual Meeting of the American Institute of Chemical Engineers, Salt Lake City, Utah, 11 November 2015.
42. "Metastabilities and Kinetics in Proteins and Viruses," Mainz Molecular Simulation Days, Max-Planck-Institute for Polymer Science, Mainz, Germany, 11 June 2015.
41. "Metastabilities and Kinetics in Proteins and Viruses," Biological Physics Seminar Series, Department of Physics, Carnegie Mellon University, 28 April 2015.
40. "Understanding and harnessing biomolecular metastabilities," Patten Seminar Series, Department of Chemical and Biological Engineering, University of Colorado, Boulder, 16 September 2014.
39. Tang-Qing Yu, Mauro Lapelosa, Eric Vanden-Eijnden, and Cameron F Abrams. "Markovian Milestoning for Computing Diffusion Rates of Ligands in Proteins," Telluride Science Research Center Workshop: Searching for Reaction Coordinates and Order Parameters, Telluride, Colorado, 11 July 2014.
38. "Understanding and harnessing biomolecular metastabilities," UW Molecular Science and Engineering Center Seminar, 22 April 2014.
37. Tang-Qing Yu, Mauro Lapelosa, Eric Vanden-Eijnden, and Cameron F Abrams. "Markovian Milestoning for Computing Diffusion Rates of Ligands in Proteins," March meeting of the American Physical Society, Denver, Colorado, 7 March 2014.
36. "Understanding and harnessing biomolecular metastabilities," Special Seminar, UC Berkeley Department of Chemical and Biomolecular Engineering, 9 January 2014.
35. "HIV-1 Envelope Structure and Function," Faculty Fellows Symposium, Drexel University, 11 November 2013.
34. "Exploring and Mapping Free Energy Surfaces using Temperature-Acceleration, the String Method, and Single-Sweep," Free Energy Calculations: Three Decades of Adventure in Chemistry and Biophysics, Snowmass, Colorado, 14-19 July 2013.
33. "MD of Soft-Matter Systems," 2013 MACH Conference, Annapolis, Maryland, 13 April 2013.
32. "Novel Microbicides against HIV," Drexel University College of Engineering, Dean's Distinguished Lecture Series, 13 February 2013.
31. "Observing Rare Events in Biomolecular Simulations using Temperature-Acceleration and the String Method," Drexel University College of Medicine, Department of Biochemistry and Molecular Biology, 26 November 2012.
30. "Observing Rare Events in Biomolecular Simulations using Temperature-Acceleration and the String Method," Physical Chemistry Seminar, University of Delaware, Dept. of Chemistry, 24 September 2012.
29. "Observing Rare Events in Biomolecular Simulations using Temperature-Acceleration and the String Method," Institut Pasteur, Montevideo, Uruguay, 3 September 2012.
28. "Collective-Variable-Enhanced Biomolecular Simulations," Kavli Institute of Theoretical Physics, UCSB, 26 April 2012.
27. "Animating the Protein Data Bank with Modern Molecular Simulations," Rutgers-Camden Center for Computational and Integrative Biology, Camden, New Jersey, 28 November 2011.

26. "Collective Variables and Conformational Sampling in Biomolecular Simulations," 2011 von Neumann Symposium of the American Mathematical Society, Snowbird, Utah, 7 July 2011.
25. "Animating the Protein Data Bank with Modern Molecular Simulations," Department of Chemical and Biomolecular Engineering, University of Pennsylvania, 6 April 2011.
24. "Target-Blind Conformational Sampling in All-Atom Protein Simulations with Temperature-Accelerated Molecular Dynamics," 240th ACS National Meeting & Exposition, Boston, Massachusetts, 25 August 2010.
23. "The Receptors for Insulin and Insulin-Like Growth Factors: All-Atom Molecular Simulations," Hagedorn Research Institute (Novo Nordisk), Gentofte, Denmark, 6 August 2010.
22. "Large-Scale Conformational Sampling in All-Atom Protein Simulations using Temperature-Accelerated Molecular Dynamics," Courant Institute Biophysics Seminar, NYU, 29 January 2010.
21. "Molecular Simulation Studies of Insulin and its Receptor," Department of Physics, Drexel University, 11 November 2008.
20. "Molecular Simulation Studies of Insulin and its Receptor," Department of Biochemistry and Molecular Biology, Drexel University College of Medicine, 28 January 2008.
19. "Molecular Simulation Studies of Chaperonin," Department of Chemical and Biomolecular Engineering, Ohio State University, 4 October 2007.
18. "Computer Simulation Studies of Chaperonin," Department of Chemical and Environmental Engineering, the University of Arizona, 28 August 2007.
17. "Some Recent Developments in Monte Carlo Simulations of Soft Condensed Matter," Department of Applied Mathematics, the University of Western Ontario, 25 October 2006.
16. "Systematic Coarse-Graining and Concurrent Multiresolution Simulation of Molecular Liquids," ORNL/CNRS NanoFocUL, 28-30 August 2006.
15. "Entanglement Effects in the Plastic Deformation of Glassy Polymers and Nanocomposites," US-Poland Workshop on Nanoscience and Nanostructured Materials, Poznan, Poland, 26-29 June 2006.
14. "Simulation Studies of Chemotaxis and Random Motility," CCNY Chemical Engineering Department, 30 January 2006
13. "Simulation Studies of Chemotaxis and Random Motility," University of New Mexico Department of Chemical and Nuclear Engineering, 6 December 2005
12. "Simulation Studies of Chemotaxis and Random Motility," Lehigh University Department of Chemical Engineering, 16 November 2005.
11. "Systematic Coarse-Graining and Concurrent Multiresolution Simulation of Molecular Liquids," University of Minnesota Institute for Mathematics and its Applications (IMA) workshop: *Effective Theories of Materials and Macromolecules*, Minneapolis, 7-11 June 2005.
10. "Simulations of Chemotaxis and Random Motility in Finite Domains," Materials Research Society Fall Meeting, Boston, 29 November 2004.
9. "Resolution Focusing in Simulations of Molecular Liquids," American Chemical Society National Meeting, Philadelphia, 22 August 2004.
8. "Resolution Focusing in Simulations of Molecular Liquids," NYU Courant Institute Applied Mathematics Seminar, 12 March 2004.
7. "Inhomogeneous Coarse-Graining of Polymers and Polymer/Metal Interfaces," FZ Jülich Workshop on Computational Soft Matter, Bonn, Germany, 9 March 2004.
6. "Multiresolution Simulation of Polymers," ETHZ Summer School on Multiscale Modeling and Simulation, Lugano, Switzerland, August, 2003.
5. "Atomistic Simulation of Energetic Fluorocarbon Ion Bombardment of Silicon," Department of Chemistry, University of Antwerp, Antwerp, Belgium, 7 December 2001.
4. "Comparison of Coarse-Graining Schemes for Structural Investigation of Polycarbonate Liquids via Simulation," Division of Engineering and Applied Science, California Institute of Technology, 9 November 2001.
3. "Theory and Simulation of the Fractal Stages of Homopolymer Collapse," Department of Physics, University of Florida, 13 Nov 2001.

2. "Molecular Dynamics Simulations of Reactive Ion Bombardment of Silicon Surfaces," Department of Physics, University of Kaiserslautern, Kaiserslautern, Germany, 10 January 2000.
1. "Molecular Dynamics Simulations of Reactive Ion Bombardment of Silicon Surfaces," Ph.D. Colloquium, Department of Chemical Engineering, University of California, Berkeley, 25 August 1999.

Contributed (speaker underlined)

80. Steven Gossert, Bibek Parajuli, Irwin Chaiken, and Cameron F. Abrams, "Roles of Variable Linker Length in Dual Acting Virucidal Entry Inhibitors on HIV-1 Potency via on-the-fly Free-Energy Molecular Simulations", Annual Meeting of the American Institute of Chemical Engineers, Pittsburgh, Pennsylvania, 30 October 2018.
79. Jasmine Gardner and Cameron F. Abrams, "Flap-Opening Dynamics and Ligand Unbinding of HIV-1 Protease Studied using Accelerated MD Simulations", Annual Meeting of the American Institute of Chemical Engineers, Pittsburgh, Pennsylvania, 30 October 2018.
78. Natasha Gupta, Ryan Gordon, Samba Somisetti, and Cameron F. Abrams, "Identifying unique HIV-1 entry inhibitor leads using virtual screening and docking techniques," American Chemical Society National Meeting, New Orleans, Louisiana, March 20, 2018.
77. Steven Gossert and Cameron F. Abrams, "Roles of Conserved Tryptophans in Trimerization of HIV-1 Membrane-Proximal External Regions: Implications for Virucidal Design via Alchemical Free-Energy Molecular Simulations", Annual Meeting of the American Institute of Chemical Engineers, Minneapolis, Minnesota, 30 October 2017.
76. Jasmine Gardner and Cameron F. Abrams, "Line Tension and Lipid Sorting Modulate Dynamics of Hemifusion Diaphragm Dissipation", Annual Meeting of the American Institute of Chemical Engineers, Minneapolis, Minnesota, 1 November 2017.
75. Jasmine Gardner and Cameron F. Abrams, "Intrinsic curvature and lipid sorting modulate dynamics of hemifusion diaphragm dissipation" 254th ACS National Meeting, Washington, DC, 20-24 August 2017.
74. Changwoon Jang and Cameron F. Abrams, "Optimizing coarse-grained potentials to improve the prediction of thermoset epoxy polymer properties" Mach Conference, Annapolis, Maryland, April 5, 2017.
73. S. Alexis Paz, Eric Vanden-Eijnden, and Cameron F Abrams. "Free energy and hidden barriers: The β-sheet structure of the prion protein," 61st Annual Meeting of the Biophysical Society, New Orleans, Louisiana, 11 February 2017.
72. Alexis Paz and Cameron F. Abrams, "Replica-Exchange on-the-Fly Parameterization: Application of a High-Precision Free-Energy Method to Understanding the Roles of the M129V/D178N Polymorphisms in the Conformational Thermodynamics of Human Prion Protein", Annual Meeting of the American Institute of Chemical Engineers, San Francisco, California, 16 November 2016.
71. Jung-ho Yang and Cameron F. Abrams, "Understanding Relationships Between Molecular Structures and Thermomechanical Properties of Thermosetting Polymers with Novel Bio-Based Building Blocks", Annual Meeting of the American Institute of Chemical Engineers, San Francisco, California, 14 November 2016.
70. Francesca Moraca, Adel A. Rashad, Kriti Acharya, Irwin Chaiken and Cameron F. Abrams, "Cyclic peptide triazoles docking and Molecular Dynamics simulation in three different gp120 states: selection of the best target for future peptide triazole's optimization", NIGMS Structural Biology Related to HIV/AIDS, Bethesda, Maryland, June 23, 2016.
69. S. Alexis Paz, Matthew Cameron, and Cameron F. Abrams, "On the Role of the V3 Loop in the Conformational Thermodynamics of Bridging Sheet Formation in HIV-1 gp120: On-the-fly parameterization Free-Energy Calculations of the BG505 SOSIP.664 protomer", NIGMS Structural Biology Related to HIV/AIDS, Bethesda, Maryland, June 23, 2016.
68. Changwoon Jang and Cameron F. Abrams, "Coarse-Grained Molecular Dynamics Simulations of DGEBA/POP-DA Crosslinked Thermosets" Mach Conference, Annapolis, Maryland, April 6, 2016.
67. S. Alexis Paz and Cameron F Abrams. "Free energy and hidden barriers: The □ -sheet structure of the prion protein," 251st National Meeting of the American Chemical Society, San Diego, California, 14 March 2016.

66. Francesca Moraca, Adel A. Rashad, Kriti Acharya, Irwin Chaiken, and Cameron F. Abrams, "Binding of the cyclic peptide triazole AAR029F to the HIV-1 envelope glycoprotein gp120 in 3 different conformations to explore its mechanism of action and the possible competition with the 17b antibody," ZING Structure-Based Drug Design Conference, San Diego, California, February 21, 2016.
65. S. Alexis Paz and Cameron F Abrams. "Prion protein conformational statistics via on-the-fly free-energy parameterization," Annual Meeting of the American Institute of Chemical Engineers, Salt Lake City, Utah, 10 November 2015.
64. Ryan Gordon and Cameron F Abrams. Aggregation of 12-Hydroxystearic Acid and its Lithium Salt in Hexane: Molecular Dynamics Simulations," Annual Meeting of the American Institute of Chemical Engineers, Salt Lake City, Utah, 9 November 2015.
63. Tang-Qing Yu, Mauro Lapelosa, Eric Vanden-Eijnden, and Cameron F Abrams. "Markovian Milestoning for Computing Rates of Entry, Exit, and Internal Diffusion of Ligands in Proteins," Biophysical Society Annual Meeting, Baltimore, Maryland, 9 February 2015.
62. Anthony Bucci and Cameron F Abrams. "Identification and Allosteric Regulation of Oxygen Pathways in Monomeric Sarcosine Oxidase Via Single-Sweep Free Energy Reconstruction," Annual Meeting of the American Institute of Chemical Engineers, Atlanta, Georgia, 17 November 2014.
61. Mauro Lapelosa, Tang-Qing Yu, Eric Vanden-Eijnden, and Cameron F Abrams. "Markovian Milestoning for Computing Diffusion Rates of Ligands in Proteins," Annual Meeting of the American Institute of Chemical Engineers, San Francisco, California, 4 November 2013.
60. Harish Vashisth and Cameron F Abrams. "Understanding the activation mechanism of the insulin receptor kinase domain using enhanced conformational sampling and free-energy calculations," Annual Meeting of the American Institute of Chemical Engineers, Pittsburgh, Pennsylvania, 29 October 2012.
59. Cameron F Abrams and Eric Vanden-Eijnden. "On the fly free energy parameterization using temperature accelerated molecular dynamics," Annual Meeting of the American Institute of Chemical Engineers, Pittsburgh, Pennsylvania, 29 October 2012.
58. Debashish Mukherji, Majid Sharifi, Guiseppe R Palmese, and Cameron F Abrams. "Toughness enhancement in neat epoxies by microsurface drawing," International Workshop on Computational Mechanics of Materials (IWCMM XXII), Baltimore, Maryland, 25 September 2012.
57. Cameron F Abrams. "Unbiased Folding of alpha-Helices using Temperature Accelerated Molecular Dynamics," Annual Meeting of the American Institute of Chemical Engineers. Minneapolis, MN, October 2011.
56. Harish Vashisth and Cameron F Abrams. "Temperature-accelerated molecular dynamics reveals that insulin can undergo large-scale conformational reorganization on binding to its receptor," Annual Meeting of the American Institute of Chemical Engineers. Minneapolis, MN, October 2011.
55. Spencer Stober and Cameron F Abrams. "Enhanced Meta-Analysis of Acetylcholine Binding Protein Structures Reveals Conformational Signatures of Agonism in Nicotinic Receptors," Annual Meeting of the American Institute of Chemical Engineers. Minneapolis, MN, October 2011.
54. Ali Emileh, Ferit Tuzer, Diogo R. Moreira, Irwin Chaiken, and Cameron F Abrams. "A model for binding of peptide-triazoledual-site antagonist entry inhibitors to HIV gp120," Gordon Research Conference on Computer Aided Drug Design, Mount Snow, VT, July, 2011.
53. Ali Emileh and Cameron F. Abrams, "HIV-1 gp120: Atomic Insight Into a Layered Topology and Plasticity of the Inner Domain," Annual Meeting of the American Institute of Chemical Engineers, Salt Lake City, Utah, November 2010.
52. Harish Vashisth and Cameron F. Abrams, "A temperature-accelerated molecular dynamics study of the insulin receptor kinase," Annual Meeting of the American Institute of Chemical Engineers, Salt Lake City, Utah, November 2010.
51. Ali Emileh and Cameron F. Abrams, "Investigation of the layered structure of HIV-1 gp120 using temperature-accelerated molecular dynamics," 24th Annual Symposium of the Protein Society, 3 August 2010, San Diego, CA.
50. Vamshi Gangupomu and Cameron F. Abrams, "Conformational prediction of the HIV-1 gp41 membrane-spanning domain," 240th ACS National Meeting & Exposition, 24 August 2010, Boston, MA.

49. Harish Vashisth and Cameron F. Abrams, "DFG-flip in the insulin receptor kinase is facilitated by a helical intermediate," 5th Protein Kinases in Drug Discovery, Boston, Massachusetts, 27 May 2010
48. Debashish Mukherji and Cameron F. Abrams, "Anomalous ductility in thermoset/thermoplastic polymer alloys: An explanation based on overlap concentration and cavity growth," MRS Spring Meeting, 5-9 April 2010, San Francisco, CA.
47. Debashish Mukherji and Cameron F. Abrams, "Possible explanation of anomalous ductility inthermoset/thermoplastic polymer alloys," APS March Meeting, 15-19 March 2010, Portland, OR.
46. Harish Vashisth and Cameron F. Abrams, "How insulin-like growth factor hormones IGF1 and IGF2 engage their cognate receptor," Biophysical Society Annual Meeting, San Francisco, CA, 22 February 2010.
45. Debashish Mukherji and Cameron F. Abrams, "Strain Hardening in Highly Cross-Linked Polymer Networks: An Explanation Based On Microvoid Formation," Annual Meeting of the American Institute of Chemical Engineers, 7-12 November 2009, Nashville TN.
44. Debashish Mukherji and Cameron F. Abrams, "Anomalous Ductility in Thermoset/Thermoplastic Polymer Alloys," Annual Meeting of the American Institute of Chemical Engineers, 7-12 November 2009, Nashville TN.
43. Ali Emileh and Cameron F. Abrams, "Investigation of geometrical constraints on α1 helix folding in b12-bound HIV-1 gp120 core through targeted molecular dynamics," Annual Meeting of the American Institute of Chemical Engineers, 7-12 November 2009, Nashville TN.
42. Harish Vashisth and Cameron F. Abrams, "Molecular Simulation Studies of Insulin Binding to the Insulin Receptor," Annual Meeting of the American Institute of Chemical Engineers, Nashville, TN, 9 November 2009.
41. Harish Vashisth and Cameron F. Abrams, "Millisecond Time-scale Ligand (Un)binding Event Studied using Accelerated Molecular Dynamics Simulations," Foundations of Molecular Modeling and Simulation (FOMMS-2009), Blaine, WA, 15 July 2009.
40. Harish Vashisth and Cameron F. Abrams, "Thermodynamics of Ligand (Un)binding in the Insulin Hexamer and the Insulin Receptor," Gordon Research Conference on Computer Aided Drug Design, Tilton, NH, 22 July 2009.
39. Debashish Mukherji and Cameron F. Abrams, "Microvoid formation and strain hardening in highly cross-linked polymer networks, American Physical Society March Meeting," 15-19 March 2009, Pittsburgh PA.
38. Harish Vashisth and Cameron F. Abrams, "A Thermodynamic Study of Ligand Access/escape from Protein Cavities," Biophysical Society Annual Meeting, Boston, MA, 4 March 2009.
37. Harish Vashisth and Cameron F. Abrams, "Docking of Insulin to its Receptor," Biophysical Society Annual Meeting, Boston, MA, 4 March 2009.
36. Harish Vashisth and Cameron F. Abrams, "Thermodynamics of Multiple Phenol Dissociation Pathways In the R6 Insulin Hexamer," Annual Meeting of the American Institute of Chemical Engineers, Philadelphia, PA, 18 November 2008.
35. Harish Vashisth and Cameron F. Abrams, "Thermodynamics of Multiple Phenol Dissociation Pathways In the R6 Insulin Hexamer," Annual Meeting of the American Institute of Chemical Engineers, Philadelphia, PA, 18 November 2008.
34. Harish Vashisth and Cameron F. Abrams, "Ligand escape pathways and free energy calculations from nonequilibrium simulations: A computational study of the insulin-phenol complex," Biophysical Society Annual Meeting, Long Beach, CA, March 2008.
33. Cameron F. Abrams, "Molecular dynamics simulations of the GroEL heptamer," Annual Meeting of the American Institute of Chemical Engineers, Salt Lake City, UT, 6 November 2007.
32. Harish Vashisth and Cameron F. Abrams, "Escape pathways of phenolic ligands from the insulin-phenol complex," Annual Meeting of the American Institute of Chemical Engineers, Salt Lake City, UT, 6 November 2007. (Co-winner, CoMSEF Graduate Student Poster Competition)
31. Yelena Sliozberg and Cameron F. Abrams, "Spontaneous conformational transitions in unbiased all-atom molecular dynamics simulations of the GroEL subunit," Biophysical Society Annual Meeting, Baltimore, MD, 6 March 2007.

30. Yelena Sliozberg and Cameron F. Abrams, "Nucleotide-dependent allostery in the GroEL subunit," Annual Meeting of the American Institute of Chemical Engineers, San Francisco, CA, November 2006.
29. Cameron F. Abrams, "Crazing and Entanglements in Glassy Polymers," FOMMS 2006, Semiahmoo, WA, 9-14 July 2006.
28. Nam-Kyung Lee, Cameron F. Abrams, and Albert Johner, "Optimal Confinement for Internal Polymer Binding" American Physical Society March Meeting, Baltimore, MD, 13 March 2006.
27. David Richardson and Cameron F. Abrams, "Entanglement Effects in Plastic Deformation of Linear Polymer Glasses," American Physical Society March Meeting, Baltimore, MD, 17 March 2006.
26. Ehsan Jabbarzadeh and Cameron F. Abrams, "Strategies to Enhance Capillary Formation inside Biomaterials: A Computational Study," 2005 Annual Meeting of the American Institute of Chemical Engineers, Cincinnati, OH, November 2005.
25. Yelena Sliozberg and Cameron F. Abrams, "Density-of-States Simulation of Collapse of Confined Heteropolymers," Annual Meeting of the American Institute of Chemical Engineers, Cincinnati, OH, November 2005.
24. David Richardson and Cameron F. Abrams, "Entanglement Effects in the Plastic Deformation of Filled Polymer Glasses: A Simulation Study," Annual Meeting of the American Institute of Chemical Engineers, Cincinnati, OH, November 2005.
23. Yelena Sliozberg and Cameron F. Abrams, "Density-of-States Simulation of Collapse of Confined Heteropolymers," American Physical Society March Meeting, Los Angeles, 2005.
22. Ehsan Jabbarzadeh and Cameron F. Abrams, "Simulation of cell chemotaxis in 2D random porous domains," Gordon Research Conference on Gradient Sensing and Directed Cell Migration, Ventura, CA, February 2005.
21. Cameron F. Abrams, "Resolution Focusing in Molecular Simulation of Liquids," 2004 Annual Meeting of the American Institute of Chemical Engineers, Austin, TX, November 2004.
20. Ehsan Jabbarzadeh and Cameron F. Abrams, "Chemotaxis and random motility in unsteady chemoattractant fields: A computational study," Annual Meeting of the American Institute of Chemical Engineers, Austin, TX, November 2004.
19. Yelena Sliozberg and Cameron F. Abrams, "Molecular simulation of branched amphiphilic heteropolymers in confined geometries," Annual Meeting of the American Institute of Chemical Engineers, Austin, TX, November 2004.
18. Ehsan Jabbarzadeh and Cameron F. Abrams, "Chemotactic Cell Migration in Inhomogeneous Domains: A Computational Study," 2004 BMES Annual Fall Meeting, Philadelphia, 16 October 2004.
17. Ehsan Jabbarzadeh and Cameron F. Abrams, "Computational Studies of Cell Migration," 30th Annual Northeast Bioengineering Conference, Springfield, MA, 2004.
16. Ehsan Jabbarzadeh and Cameron F. Abrams, "Computational Studies of Cell Migration," 17th Annual Mid-Atlantic Biochemical Engineering Meeting, University of Maryland, Baltimore County, 2004.
15. Yelena Sliozberg, Nam-Kyung Lee, and Cameron F. Abrams. "Molecular Dynamics Simulation of Intramolecular Self-Assembly in Polysoaps", Annual Meeting of the American Institute of Chemical Engineers, San Francisco, California, November 2003.
14. Cameron F. Abrams, Luigi Delle Site, and Kurt Kremer. "Multiscale Molecular Dynamics Simulation of the Liquid Polycarbonate/Nickel (111) Interface," Materials Research Society Fall Meeting 2002, Boston, MA, 2-6 December 2002.
13. Cameron F. Abrams, Nam-Kyung Lee, and Sergei Obukhov. "A Combined Simulation and Theoretical Study of Homopolymer Collapse," Annual Meeting of the American Institute of Chemical Engineers, Indianapolis, Indiana, 3-8 November 2002.
12. Cameron F. Abrams and Kurt Kremer. "Multiscale Simulation of Bisphenol-A-Polycarbonate," CIMTEC 2002, 3rd Forum on New Materials, Florence, Italy, 14-18 July 2002.
11. Cameron F. Abrams and Kurt Kremer. "Structure and Dynamics of Polycarbonate Melts via Novel Coarse-Grained Molecular Dynamics Simulation," Annual Meeting of the American Institute of Chemical Engineers, Reno, Nevada, 4-9 November 2001.

10. Cameron F. Abrams and David B. Graves. "Product Formation Mechanisms in Fluorocarbon Ion Etching of Silicon via Atomistic Simulation," Annual Meeting of the American Institute of Chemical Engineers, Reno, Nevada, 4-9 November 2001.
9. V. V. Serikov, S. Kawamoto, Cameron F. Abrams, and David B. Graves. "Atomic scale simulation of plasma-assisted deposition of diamond-like carbon films," 22nd International Symposium on Rarefied Gas Dynamics, Syndey, Australia, 9-14 July 2000.
8. Cameron F. Abrams and David B. Graves. "Deposition and Etching Using Fluorocarbon Ions: Molecular Dynamics Simulations," Annual Meeting of the American Institute of Chemical Engineers, Dallas, Texas, 31 October - 5 November 1999.
7. Cameron F. Abrams and David B. Graves. "Deposition and Etching Using Fluorocarbon Ions: Molecular Dynamics Simulations," 46th International Symposium of the American Vacuum Society, Seattle, Washington, 25-29 October 1999.
6. Junichi Tanaka, Cameron F. Abrams, and David B. Graves. "Molecular Dynamics Simulations of Fluorocarbon Films," 46th International Symposium of the American Vacuum Society, Seattle, Washington, 25-29 October 1999.
5. Cameron F. Abrams and David B. Graves. "Scattering and Sputtering Processes of Energetic Ar^+ and Cu^+ Ions on Cu Surfaces: Molecular Dynamics Simulations," 45th International Symposium of the American Vacuum Society, Baltimore, Maryland, 2-6 November 1998.
4. Cameron F. Abrams and David B. Graves. "Scattering and Sputtering Processes of Energetic Ar^+ and Cu^+ Ions on Cu Surfaces: Molecular Dynamics Simulations," 51st Annual Gaseous Electronics Conference of the American Institute of Physics, Maui, Hawaii, 19-22 October 1998.
3. Cameron F. Abrams and David B. Graves. "Molecular Dynamics Simulations of Ar^+ and Cu^+ Impacts onto Cu Surfaces: Product Spatiokinetic Distributions," Northern California Chapter of the American Vacuum Society Thin Films User Group Symposium, Foster City, California, 12 October 1998.
2. Cameron F. Abrams and David B. Graves. "Scattering and Sputtering Processes of Energetic Ar^+ and Cu^+ Ions on Cu Surfaces: Molecular Dynamics Simulations," Gordon Research Conference on Plasma Processing Science, Tilton School, New Hampshire, 9-14 August 1998.
1. Cameron F. Abrams and David B. Graves. "Energy and Angular Distributions of Argon Ions Reflected from SiO_2 Surfaces: Molecular Dynamics Simulations," 44th International Symposium of the American Vacuum Society, San Jose, California, 20-24 October 1998.

Funded Proposals (CFA is PI unless otherwise indicated; all Co-I's are listed where applicable; * = active project as of March, 2018; $6.25MM as PI, $34.4MM total)

23. *"Transition Path Theory and Markovian Milestoning for Prediction of Protein-Ligand Binding Kinetics in Molecular Simulations," NIH R01 GM100472 (1st renewal), 9/1/17-5/31/21, $1,300,000, PI. (Co-I: Eric Vanden-Eijnden, NYU).
22. *"Thermosets for Agile Manufacturing," W911NF-17-2-0227, Army Research Lab $3,000,000, Co-I (PI: G. R. Palmese). 9/1/17-8/31/20. Abrams' share supports one FTE PhD student and ½ of a postdoc.
21. *"Biobased Thermosetting Polymers for Composite, Adhesive, and Coating Applications," Army Research Lab W911NF-12-R-0011 $2,400,000, Co-I (PI: G. R. Palmese). 1/1/17-12/31/19. Abrams' share supports one FTE PhD student.
20. "Dual-action virolytic entry inhibitors against HIV-1", NIH R01 GM115249 $1,700,000, Co-PI (Multiple-PI grant; other Co-PI is Irwin Chaiken, DUCOM). 7/1/15-6/30/19. Abrams' share supports one FTE PhD student.
19. *" Structure-based antagonism of HIV-1 envelope function in cell entry", NIH P01 GM056550 $10,000,000, Co-I (PI: I. Chaiken) 9/30/13-8/31/18. Abrams is the leader of the Computational Core of this program project, directly supervising one postdoc and an annual direct cost of $70,000.
18. "Drexel/ExxonMobil Sponsored Research Agreement: Advanced Studies of Self-Assembly", $460,000, 1/1/14-12/31/17.
17. "Center for Sustainable Corrosion Protection," Army Research Lab W911NF-13-2-0046, $3,000,000, Co-I (PI: G. R. Palmese), 9/1/13-8/31/18.

16. "Collaborative Research: Multiscale molecular simulations of protein-mediated bilayer fusion," NSF Award Number MCB-1330205, $350,000, PI, 9/1/13-8/31/18. This is a collaboration with M. Deserno at CMU; CMU budget is also $350,000, but does not pass through Drexel.
15. "Collaborative Research: On-the-fly free energy parameterization in molecular simulations", NSF Award Number DMR-1207389, $286,455, 9/1/12-8/31/15. NYU (Vanden-Eijnden) is the secondary institution, receiving about the same amount.

Prior to promotion to Full Professor

14. *"Materials in Extreme Dynamic Environments: The Johns Hopkins Consortium", US Army Award Number W911NF-12-2-0022, Total Amount Unknown; CFA's share approx. $75,000 per year for four years (PI: KT Ramesh, JHU).
13. "Approaches to computing diffusion rates in proteins from transition path theory," NIH R01 GM100472, 9/1/11-5/31/16, $1,100,000, PI. (Co-I: Eric Vanden-Eijnden, NYU).
12. "PASI: Molecular-Based Multiscale Modeling and Simulation; Montevideo, Uruguay; September 1-14, 2012", NSF Award Number OISE-1124480, $100,000 (PI: James Pfaendtner, UW).
11. "HIV-1 gp120 conformational transitions in activation and antagonism, NIH Award Number 1 R21 AI 093248, 4/1/11-3/31/13, $450,000, Co-PI (Multiple-PI grant; other Co-PI is Irwin Chaiken, DUCOM Biochemistry).
10. "Conformational signatures of Neurotransmitter-Induced Gating and Desensitization of Nicotinic Ion Channels: A Collaborative Simulation and Experimental Approach," Commonwealth of Pennsylvania, Tobacco Settlement Funds, GRID/CURE, 1/1/11-12/31/11, $55,000; (Co-I: Mike White, DUCOM Biochemistry).
9. "MRI: Acquisition of a GPU-Accelerated High Performance Computing Cluster," National Science Foundation, Award Number AST-0959884, 3/1/10-2/28/11, $440,000 (PI: Steve McMillan, DU Physics; Co-I's Jeremy Johnson and Naga Kandasamy).
8. "Chimeric Virucides Based on a Novel Theory of Viral Metastability," NIH Award Number 5 R01 AI 084117, 9/1/09-8/31/13, $1,300,000. (Co-I Irwin Chaiken, DUCOM Biochemistry).

Prior to tenure

7. "DURIP: Acquisition of a High-Performance Computer Cluster," US Army, Award Number W911NF-07-1-0301, $120,000, 6/15/07-6/14/08.
6. "Drexel-ARL Materials Center of Excellence in Polymeric Materials," US Army, Award Number W911NF-06-2-0013, $1,350,000 (20% of $6,750,000), 3/30/2006-3/31/2011 (PI: Giuseppe Palmese; Co-I's Yossef Elabd and Chris Li)
5. "CAREER: Multiscale simulation of solute transport in hydrogels," NSF, Award Number CBET-0544933, $400,000, 2/1/2006-1/31/2010.
4. "Thermodynamics of Heteropolymers in Confinement," American Chemical Society, Award Number PRF 42368-G7, $35,000, 2/2005-1/2007.
3. "ITR: Inhomogeneously Resolved Simulation of Protein Assembly Dynamics," NSF, Award Number DMR-0427643, $420,000, 9/2004-8/2008.
2. "Predicting Failure in Carbon Nanotube Reinforced Polymer Composites: A Novel Multiscale Simulation Approach," Office of Naval Research Young Investigators Program, Award Number N00014-03-1-0655, $332,313, 6/2003-5/2006.
1. "QSB: Quantitative Simulation of Cell Migration in Porous Biomaterials," NSF, Award Number CBET-0331191, $96,129, 11/2003-10/2005.

Supercomputer Time (Approx. 7 Million Hours)

3. *"Molecular Dynamics Studies of Epoxies," DoD HPCMP, 6M hours, through 9/30/2019.
2. *"Molecular Dynamics Studies of Various Protein Systems," NSF XSEDE, 7/1/2007-present, Grant No. MCB070073N.

1. "Molecular Simulation of Mechanical Deformation of Filled Epoxies," NSF TeraGrid, 30,000 hours, 9/1/2006-9/1/2007, Grant No. DMR060052T.

Pending/Planned (as of September, 2019)

1. "Dual-action virolytic entry inhibitors against HIV-1", NIH R01 GM115249 $1,700,000, Co-PI (Multiple-PI grant; other Co-PI is Irwin Chaiken, DUCOM). 7/1/15-6/30/19. Abrams' share supports one FTE PhD student.

Patent

1. Cameron F. Abrams, Irwin M. Chaiken, Mark R. Contarino, Bibek Parajuli and Adel Ahmed Rashad Ahmed. Novel Compositions for Promoting HIV-1 Virolysis and Methods Using Same. US Patent 9,233,138, January 6, 2016.

Students Supervised (*current group members; underline denotes graduates; 11 PhD graduates as of Sept, 2019)

Ph.D.

18. *Ming Huang, "Molecular Simulations of Thermoset Additive Manufacturing," Dates of supervision: 11/17-present.
17. Matthew Cameron, "Milestoning MD of Ligand Binding Kinetics," Dates of supervision: 11/16-8/17. Left PhD program.
16. Donald Seaman, "Molecular Simulations of Bio-based Thermosets," Dates of supervision: 11/16-6/19. Left PhD program. Supported by W911NF-12-R-0011.
15. *Natasha Gupta, "Computational Design of HIV-1 Entry Inhibitors," Dates of supervision: 11/16-present. Supported by Janssen Pharmaceuticals.
14. *Steven Gossert, "Novel HIV-1 Virucides," Dates of supervision: 11/15-present. Supported on NIH GM115249.
13. Dr. Jasmine Gardner, "Bilayer fusion and advanced rate calculation methods," Dates of supervision: 11/14-6/19. Supported on NSF MCB-1330205. Now a Postdoc at Uppsala University, Sweden.
12. Dr. Arun Srikanth, "Molecular simulations of thermosets," Dates of supervision: 11/13-06/18. Supported on W911NF-13-2-0046. Now a postdoc at the University of Bath, UK.
11. Dr. Ryan Gordon, "Molecular Simulation Studies Self-Assembly," Dates of Supervision: 11/13-06/18. Supported on ExxonMobil SRA. Now at Lockheed Martin.
10. Dr. Anthony Bucci, "Approaches to computing diffusion rates in proteins using transition-path theory," Dates of supervision: 10/11-5/16. Supported on NIH R01 GM 100472. Currently employed at West Pharma.
9. Dr. Michelle Baker, "Molecular Simulation Studies of HIV-1 Structural Biology," Dates of Supervision: 9/09-8/14. Supported on NIH R01 AI 084117 and NSF DMR-1207389. Currently employed at Johnson&Johnson.
8. Dr. Ali Emileh, "Molecular Simulation of HIV-1 gp120," Dates of supervision: 10/07-12/12. Supported on NIH R21 AI 093248. Currently Scientist III at BASF Enzymes, San Diego.
7. Dr. Spencer Stober, "Protein Conformational Changes," Dates of supervision: 1/08-9/12. Support: Part-time PhD, self-supporting (ExxonMobil); Dean's Fellowship: 1/09-1/11; GRID/CURE 1/11-9/12. Currently at ExxonMobil Central Strategic Research.
6. Dr. Vamshi Gangupomu. "Molecular Simulations Studies of HIV-1 gp41 Protein-Membrane Interactions," Dates of supervision: 7/09-10/10 (previously supervised by Franco Capaldi, MEM). Graduated October 2010. Supported on NIH R01 AI 084117. Currently a consulting engineer for Total Validation Services Inc.
5. Dr. Harish Vashisth. "Molecular Dynamics Studies of Insulin." Dates of Supervision: 9/05-6/10. Graduated, June 2010. Supported on NSF CBET-0544933 (CAREER). Currently an associate professor with tenure in the Chemical Engineering Department and the University of New Hampshire.
4. Daniel Rundle. Dates of supervision: 9/05-6/06. Left PhD program.

3. David G. Richardson (co-advisor: W. Krandick, Drexel CS). Dissertation title unknown. Dates of supervision: 10/03-10/06. Supported on ONR N00014-03-1-0655. Graduation date unknown.
2. Dr. Yelena Sliozberg. "Molecular Simulation of Chaperonins," Dates of Supervision: 9/02-9/07. Graduated, September 2007. Supported on startup funds (including a Glick Fellowship), ACS PRF 42368-G7 (270082), and NSF DMR-0427643. Currently on staff at Army Research Lab.
1. Dr. Ehsan Jabbarzadeh (co-advisor: C. Laurencin, UVA). "Theoretical and Experimental Approaches to Vascularization of Tissue Engineered Bone," Dates of supervision: 1/03-6/07; Graduated, June 2007. Winner of the "Best Doctoral Dissertation in the Physical and Mathematical Sciences", 2007. Winner of a College of Engineering Hill Fellowship, 2007. Supported on startup funds, NSF CBET-0331191, UVA Subcontract. Currently an associate professor with tenure in the Chemical Engineering Department and the University of South Carolina.

Post-docs

10. *Dr. Mohammadjavad Mohammadi, "Computational Drug Design of HIV-1 Entry Inhibitors," Dates of supervision: 2019-present. Supported on NIH P01 GM056550.
9. *Dr. Gourav Shrivastav, "Markovian Milestoning," Dates of supervision: 2018-present. Supported on NIH R01 GM 100472.
8. *Dr. Salman Zarrini, "Molecular Simulation Studies of Thermosets," Dates of supervision: 2018-present. Supported on US Army W911NF-13-2-0046.
7. Dr. Samba Venkatasomisetti, "Computational Drug Design of HIV-1 Entry Inhibitors," Dates of supervision: 2017-2019. Supported on NIH P01 GM056550.
6. Dr. Jungho Yang, "Computational Studies of Corrosion," Dates of supervision: 2015-2017. Supported on US Army W911NF-13-2-0046. Currently Post-Doc at Ohio State University.
5. Dr. Francesca Moraca, "Computational Drug Design of HIV-1 Entry Inhibitors," Dates of supervision: 2014-2016. Supported on NIH P01 GM056550.
4. Dr. Sergio Alexis Paz, "On-the-fly free energy parameterization," Dates of supervision: 2014-2016. Supported on NSF DMR-1207389. Currently an assistant professor in the Department of Chemistry at the National University of Córdoba in Argentina.
3. Dr. Chang-Woon Jang, "Molecular Simulations of Epoxies," Dates of supervision: 2012-2017. Supported on US Army Award W911NF-12-2-0022. Currently postdoc at Nagoya University, Japan.
2. Dr. Mauro Lapelosa, "Transition-Path Theory," Dates of supervision: 2011-2013. Supported on NIH R01 GM 100472.
1. Dr. Debashish Mukherji, "Molecular simulations of epoxies," Dates of supervision: 2008-2010. Supported on US Army Award W911NF-06-2-0013. Currently at MPIP.

Masters

1. Shyno Mathew, MS. "Studies of O_2 diffusion in monomeric sarcosine oxidase", Dates of supervision: 6/08-6/10. Graduated BS/MS June 2010. Currently PhD student in Chemical Engineering at Columbia University.

Undergraduates

8. Ariel Yeung, "Molecular Simulations in HIV," 2019-present.
7. Tapiwanahse Ndlovu, "Computational exploration of EGFRK," 2015-2016.
6. Stephanie Edwards, "Computational exploration of HIV-1 Env drug design targets," 2014-2015.
5. Matthew Cameron, "Computational drug design of HIV-1 entry inhibitors," 2014-2016.
4. Priya Ramachandrula, "Enhanced Sampling MD of Calmodulin," Summer STAR, 2013; 2015-2016.
3. Charles Bender, "2-D Wang-Landau Monte Carlo," Summer STAR, 2004.
2. Christopher Petersen, "2-D Wang-Landau Monte Carlo," Summer STAR, 2004
1. Suroor Manzoor, "Bitwise Voxelized 3D Domains: Toward Efficient Simulation of Diffusion in Porous Media," 2/2003-7/2003.

Honors and Awards

16. Department of Chemical and Biological Engineering Research Award (Drexel University), 2017
15. Impact Award in Computational Molecular Science and Engineering, American Institute of Chemical Engineers, 2015
14. Fellow, American Institute of Medical and Biological Engineering, 2015
13. College of Engineering Research Award (Drexel University), 2014
12. Invited Participant, "Physical Principles of Multiscale Modeling, Analysis and Simulation in Soft Condensed Matter," Kavli Institute for Theoretical Physics, UCSB, 4/15/2012-5/4/2012
11. General Participant, National Academy of Engineering "German-American Frontiers of Engineering" Symposium, 2008
10. Graduate Mentor of the Year, 2007 (Drexel University)
9. NSF CAREER, 2006
8. General Participant, National Academy of Engineering "Frontiers of Engineering" Symposium, 2004
7. Office of Naval Research Young Investigator, 2003-2006
6. Chevron Graduate Fellow, University of California, Berkeley, Dept. Chem. Engr., 1998
5. 2nd Place, Poster Competition, 1998 Northern California AVS Thin Films User Group
4. 1st Place, 1995 AIChE Southern Regional Undergraduate Paper Contest
3. 3rd Place, 1994 AIChE Southern Regional Undergraduate Paper Contest
2. Phi Kappa Phi Inductee, 1991
1. Kodak (Eastman) Scholar, 1991

Service

Department of Chemical and Biological Engineering, Drexel University

1. Chair, Graduate Committee, 2008-2014 (Member 2008-present)
2. Member, Undergraduate Committee, 2008-present
3. Member, Committee on Academic Standing, 2008-2017; Chair, 2014-2017
4. Graduate Advisor, 2008-2014
5. Standing Member, Faculty Search Committee
6. Standing Member, Faculty Evaluation Committee
7. Faculty Advisor, AIChE Student Chapter, 2004-2006
8. Seminar series organizer, 2003-2006
9. Department Head, 2017-present

College of Engineering, Drexel University

1. Member, Junior Advisory Committee, 2006-2008
2. Member, Senior Advisory Committee, 2008-2010
3. Member, Tenure and Promotion Committee, 2015-2017
4. Member, Task Force on Computational Engineering Minor, 2015-2016
5. Chair, Electrical and Computer Engineering Department Head Search Committee, 2018

University

1. Workshop tutor, Drexel Center for Academic Excellence, 2002-2003
2. Scholars Day Interviewer, 2003 & 2005
3. Open Houses (several)
4. Member of the Faculty Senate representing COE, 2010-2013
5. Member, COE Dean's Search Committee, 2010-2011 (Search failed)
6. Member, Senate Committee on Research and Scholarly Activities, 2010-2013. Chair, 2011-2013
7. Member, Strategic Initiative #4 Implementation Task Force, 2012-2013
8. Member, Computing Task Force, 2012-2013
9. Chair, Board of Governance of the University Research Computing Facility, 2013-present
10. Member, Lebow College of Business Dean's Search Committee, 2012-2014; Hired Frank Linnehan
11. Member, CIO Search Committee, 2015; Hired Tom DiChiaro.
12. Provost's Fellow, CY 2016, under SVPR Aleister Saunders.

13. Member, Review Committee for CoE Dean Joseph Hughes, 2016.

Profession

1. National member: AIChE, ACS, APS, Biophysical Society, AIMBE
2. Session Chair, AIChE Annual Meetings, 2004-2011
3. Session Chair, ACS Annual Meeting, 2016
4. Session Co-organizer, APS March Meeting, 2004
5. Session Organizer, APS March Meeting, 2005:
   a. "Theory and Simulation of Polymers I: General"
   b. "Theory and Simulation of Polymers II: Surfaces and Confinement"
6. Ad-hoc Proposal Reviewer (counts): NSF (18), ACS (4), NIH (1), ESF (1), DTRA (1), AVH (1), ISF (1)
7. Review Panelist (counts): NSF (9), NIH (9)
8. Site visit panel: NSF-STC (1, Chair)
9. Referee for the following journals (counts as of March 2019; 163 total):

Acta Biochemica et Biophysica Sinica (1)
Applied Physics Letters (2)
Applied Surface Science (1)
BBA Biomembranes (1)
Biomacromolecules (1)
Biophysical Journal (2)
Biopolymers (1)
Chemical Physics (1)
Chemical Physics Letters (4)
Chemistry of Materials (1)
ChemMedChem (3)
Clinical and Vaccine Immunology (1)
Colloids and Surfaces: B (1)
Composites Science and Technology (1)
Computational Biological Chemistry (2)
Computational Materials Science (2)
Entropy (2)
European Polymer Journal (1)
Europhysics Letters (1)
Fluid Phase Equilibria (1)
Future Medicinal Chemistry (3)
Industrial and Engineering Chemistry Research (4)
Journal of the American Chemical Society (4)
Journal of Applied Physics (1)
Journal of Chemical Information and Modeling (1)
Journal of Chemical Physics (14)
Journal of Chemical Theory and Computation (10)
Journal of Computational Chemistry (1)
Journal of Energetic Materials (1)
Journal of Molecular Graphics and Modeling (3)
Journal of Molecular Catalysis B- Enzymes (1)
Journal of Physical Chemistry B (16)
Journal of Polymer Science B (6)
Journal of Statistical Physics (1)
Journal of Theoretical Biology (1)
Journal of Vacuum Science and Technology B (1)
Journal of Virology (1)
Langmuir (1)
Macromolecular Theory and Simulation (1)
Macromolecules (11)
Molecular Membrane Biology (2)
Molecular Simulation (4)
Multiscale Modeling and Simulation (1)
Nature Communications (1)
Nuclear Instruments & Methods B (1)
Physical Chemistry Chemical Physics (5)
Physical Review E (7)
Physical Review Letters (9)
Physical Review X (1)
PLoS One (3)
Polymer (1)
Proceedings of the National Academy of Sciences (2)
Proteins (2)
RSC Advances (1)
SMAI Journal of Computational Mathematics (1)
Scientific Reports (2)
Soft Matter (3)

New Courses Developed

CHE 800-002: Molecular Simulation (2003-04 Spring Term)
Fundamentals of statistical mechanics, simulation programming and execution, Molecular Dynamics and Monte Carlo methods, free energy techniques, and advanced special topics (transition path sampling and Wang-Landau MC) were all covered in this course. Extensive course web pages were developed and continue

to be maintained as a reference (www.pages.drexel.edu/~cfa/msim/). Students were evaluated based on individual term projects.

CHE 206: Basic Chemical Engineering Thermodynamics (2007-08 Winter and all Winter/Summer terms)
This is the first of a two-course sequence in thermodynamics for chemical engineering majors, and it replaces general engineering thermodynamics (TDEC 210 or "Energy II"). Text is *Chemical, Biochemical and Engineering Thermodynamics* by S. Sandler.

CHE 614: Advanced Graduate Chemical Engineering Thermodynamics (2010-11 Fall Term)
This is a new course in statistical mechanics for PhD students in Chemical Engineering. Students were evaluated based on homework assignments, two exams, and a term project. Text is *Introduction to Modern Statistical Mechanics* by D. Chandler.

ENGR 131: Introductory Programming for Engineers (2018-19 Winter Term)
This course used a zyBooks platform to teach Python to freshman engineering students. The lead instructor was Naga Kandasamy (Drexel ECE). Abrams lectured to one of four sections and developed the two take-home programming assignments.