# Cameron F. Abrams, PhD

Department of Chemical and Biological Engineering
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## EDUCATION

**B.S.**, Chemical Engineering — North Carolina State University 1995

**Ph.D.**, Chemical Engineering — University of California, Berkeley 2000
*Molecular Dynamics Simulations of Plasma-Surface Chemistry*
Committee: David Graves (chair), Arup Chakraborty, Martin Head-Gordon

## PROFESSIONAL EXPERIENCE

**Drexel University** — Department of Chemical and Biological Engineering
- Bartlett-Barry Professor of Chemical and Biological Engineering 2021-
- 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**
- Postdoc, Theory 2000-2002

**University of California, Berkeley** — Department of Chemical Engineering
- Graduate Research Assistant 1995-2000
- Graduate Teaching Assistant 1995-1997

**North Carolina State University** — Departments of Chemical Engineering & Computer Science
- Undergraduate Teaching Assistant 1993-1995

**Eastman Chemical**
- Summer Intern 1994

**Dupont, Dacron Technical Research Lab**
- Co-op Engineer (3 1-semester rotations) 1991-1993

## ADMINISTRATIVE HIGHLIGHTS

**Head, Department of Chemical and Biological Engineering** — Drexel University 2017-
- TT Hires: 4; NTT Hires: 3; Tenure cases: 4 (100%); Promotion cases: 4 (100%)
- Development: 2 $2M gifts for chaired professorships; $100k endowed research fund; $60k gift package for undergraduate lounge; $2M in endowed PhD funds
- ~$10k/y discretionary expenditure to support undergraduate experience
- $6M in capital investment from University for research lab renovation

**Inaugural Chair, Drexel University Research Computing Facility** — Drexel University 2013-2017
- Developed governance model
- Assembled first governing board and hired staff
- Secured $1.1M in university funds for seed cluster

## PUBLICATIONS

138. Shilei Ding, Derek Yang, Irfan Ullah, Ling Niu, Matthew Unger, Marco Díaz-Salinas, Monika Chandravanshi, Fei Zhou, Guillaume Beaudoin-Bussières, Mehdi Benlarbi, William Tolbert, Keon-Woong Yoon, Ruixue Xu, Geneviève Laroche, Fleur Gaudette, Abraham Morton, Zabrina Lang, Anna Son, **Cameron F. Abrams**, Marceline Côté, Amos Smith III, Rick Huang, Doreen Matthies, James Munro, Marzena Pazgier, Pradeep Uchil, Andrés Finzi (2025). “Optimization

of VE607 to generate analogs with improved neutralization activities against SARS-CoV-2 variants." *Journal of Virology* **99**, e01034-25. doi:10.1128/jvi.01034-25 PMID:41081594

137. Salsabil Abou-Hatab, **Cameron F. Abrams** (2025). "Minimal Collective Variables for Conformational Transitions in Steered and Temperature-Accelerated MD Simulations: A T4 Lysozyme Case Study." *Journal of Physical Chemistry B* **129**, 5176-5188. doi:10.1021/acs.jpcb.5c01129 PMID:40375602
136. Bibek Parajuli, Kriti Acharya, Harry Bach, Shiyu Zhang, **Cameron F. Abrams**, Irwin Chaiken (2025). "Monovalent Lectin Microvirin Utilizes Hydropathic Recognition of HIV-1 Env for Inhibition of Virus Cell Infection." *Viruses* **17**, 82. doi:10.3390/v17010082 PMID:39742730
135. Mehdi Benlarbi, Shilei Ding, Étienne Bélanger, Alexandra Tauzin, Raphael Poujol, Halima Medjahed, Omar El Ferri, Yuxia Bo, Catherine Bourassa, Julie Hussin, Judith Fafard, Marzena Pazgier, Inès Levade, **Cameron F. Abrams**, Marceline Côté, Andrés Finzi (2024). "Temperature-dependent Spike-ACE2 interaction of Omicron subvariants is associated with viral transmission." *mBio* **15**, e0090724. doi:10.1128/mbio.0097-24 PMID:39791898
134. Monisha Gupta, Gabriela Canziani, Charles Ang, Mohammadjavad Mohammadi, **Cameron F. Abrams**, Derek Yang, Amos B. Smith, III, Irwin Chaiken (2023). "Pharmacophore Variants of the Macrocyclic Peptide Triazole Inactivator of HIV-1 Env." *Med. Chem. Res.* **32**, 1497-1509. doi:10.1007/s00044-023-03092-0 PMID:39790932
133. Shilei Ding, William D. Tolbert, Huile Zhu, Daniel Lee, Tyler Higgins, Xuchen Zhao, Dung Nguyen, Rebekah Sherburn, Jonathan Richard, Gabrielle-Gendron Lepage, Halima Medjahed, Mohammadjavad Mohammadi, Cameron Abrams, Marzena Pazgier, Amos B. Smith III, Andrés Finzi (2023). "Piperidine CD4-mimetic compounds expose vulnerable Env epitopes sensitizing HIV-1-infected cells to ADCC." *Viruses* **15**, 1185. doi:10.3390/v15051185 PMID:37243271
132. Christopher Fritcshi, Saumya Anang, Zhen Gong, Mohammadjavad Mohammadi, Jonathan Richard, Catherine Bourassa, Kenny T. Severino, Hannah Richter, Derek Yang, Hung-Ching Chen, Ta-Jung Chiu, Michael S. Seaman, Navid Madani, **Cameron F. Abrams**, Andrès Finzi, Wayne A. Hendrickson, Joseph Sodroski, Amos B. Smith, III (2023). "Indoline CD4-mimetic Compounds Mediate Potent and Broad HIV-1 Inhibition and Sensitization to Antibody-dependent Cellular Cytotoxicity." *Proc. Natl. Acad. Sci. USA* **120**, e2222073120. doi:10.1073/pnas.222073120 PMID:39435159
131. Giulio Alberini, S. Alexis Paz, **Cameron F. Abrams**, Fabio Benfenati, Luca Maragliano (2023). "Molecular Dynamics Simulations of Ion Permeation in Human NaV Channels." *J. Chem. Theory. Comput.* **19**, 2953-2972. doi:10.1021/acs.jctc.2c00990 PMID:37116214
130. Ming Huang, **Cameron F. Abrams** (2023). "HTPolyNet: A general system generator for all-atom molecular simulations of amorphous crosslinked polymers." *SoftwareX* **21**, 101303. doi:10.1016/j.softx.2022.101303
129. Cheyenne Chaplain, Christopher Fritschi, Saumya Anang, Zhen Gong, Jonathan Richard, Shuaiyi Yang, Mohammadjavad Mohammadi, Jun Park, Andrés Finzi, Navid Madani, Joseph Sodroski, **Cameron F. Abrams**, Wayne Hendrickson, Amos B. Smith, III (2022). "Structural and Functional Characterization of Indane-core CD4-mimetic Compounds Substituted with Heterocyclic Amines." *ACS Med. Chem. Lett.* **14**, 51-58. doi:10.1021/acsmedchemlett.2c00376 PMID:36655122
128. Natasha Gupta Vergara, **Cameron F. Abrams** (2022). "Entropic overcompensation of the N501Y mutation on SARS-CoV-2 S binding to ACE2." *J. Chem. Inform. Model.* **63**, 633-642. doi:10.1021/acs.jcim.2c01246 PMID:36584335
127. Shilei Ding, Irfan Ullah, Shang Yu Gong, Jonathan R. Grover, Mohammadjavad Mohammadi, Yaozong Chen, Dani Vézina, Guillaume Beaudoin-Bussières, Vijay Tailor Verma, Guillaume Goyette, Fleur Gaudette, Jonathan Richard, Derek Yang, Amos B. Smith III, Marzena Pazgier, Marceline Côté, **Cameron F. Abrams**, Priti Kumar, Walther Mothes, Pradeep D. Uchil,

Andrés Finzi, Christian Baron (2022). “VE607 stabilizes SARS-CoV-2 Spike in the ‘RBD-up’ conformation and inhibits viral entry.” *iScience* **25**, 104528. doi:10.1016/j.isci.2022.104528 PMID:35233570

126. Ming Huang, Nicolas Alvarez, Giuseppe Palmese, Cameron Abrams (2022). “The Effect of Network Topology on Material Properties in Vinyl-ester/Styrene Thermoset Polymers using Molecular Dynamics Simulations and Time-Temperature Superposition.” *Comput. Mater. Sci.* **27**, 111264. doi:10.1016/j.commatsci.2022.111264
125. Salman Zarrini, Cameron Abrams (2022). “Modeling sizing emulsion droplet deposition onto silica using all-atom molecular dynamics simulations.” *Composites Part B: Engineering* **235**, 109712. doi:10.1016/j.compositesb.2022.109712
124. Christopher Fritschi, Shuaiyi Liang, Mohammadjavad Mohammadi, Saumya Anang, Francesca Moraca, Junhua Chen, Navid Madani, Joseph Sodroski, Cameron Abrams, Wayne Hendrickson, Amos Smith, III (2021). “Identification and Validation of gp120 Residue His105 as a Novel Target for HIV-1 Neutralization by Small-Molecule CD4-Mimics.” *ACS Med. Chem. Lett.* **12**, 1824-1831. doi:10.1021/acsmedchemlett.1c00437 PMID:34795873
123. Ketan Khare, Cameron Abrams (2021). “Atomistic Simulation of Volumetric Properties of Epoxy Networks: Effect of Monomer Length.” *Soft Matter* **17**, 9957-9986. doi:10.1039/D1SM01128F PMID:34698327
122. Sergio Ribone, Sergio Alexis Paz, Cameron Abrams, Marcos Villarreal (2021). “Target identification for repurposed drugs active against SARS-CoV-2 via high-throughput inverse docking.” *J. Comput. Aided Mol. Des.* **26**, 1-13. doi:10.1007/s10822-021-00432-3 PMID:34825285
121. Jérémie Prévost, Jonathan Richard, Romain Gasser, Shilei Ding, Clément Fage, Sai Priya Anand, Damien Adam, Natasha Gupta Vergara, Alexandra Tauzin, Mehdi Benlarbi, Shang Yu Gong, Guillaume Goyette, Anik Privé, Sandrine Moreira, Hugues Charest, Michel Roger, Walther Mothes, Marzena Pazgier, Emmanuelle Brochiero, Guy Boivin, **Cameron F. Abrams**, Arne Schön, Andrés Finzi (2021). “Impact of temperature on the affinity of SARS-CoV-2 Spike for ACE2.” *J. Biol. Chem.* **297**, 101151. doi:10.1016/j.jbc.2021.101151 PMID:34478710
120. S. Zarrini, C. F. Abrams (2021). “The Roles of Coupling Agent and Surfactant in Droplet Structure in Sizing Emulsions: A Molecular Dynamics Simulations Study.” *Langmuir* **37**, 10183-10190. doi:10.1021/acs.langmuir.1c01592 PMID:34396774
119. C. G. Ang, E. Carter, A. Haftl, S. Zhang, A. A. Rashad, M. Kutzler, C. F. Abrams, I. M. Chaiken (2021). “Peptide triazole thiol irreversibly inactivates metastable HIV-1 Env by accessing conformational triggers intrinsic to virus-cell entry.” *Microoganisms* **9**, 1286. doi:10.3390/microorganisms9061286 PMID:34204725
118. G. Shrivastav, C. F. Abrams (2021). “Optimizing string method’s reproducibility using generalized solute tempering replica exchange.” *J. Phys. Chem. B* **125**, 6609-6616. doi:10.1021/acs.jpcb.1c02143 PMID:34110824
117. A. Gaffney, A. Nangarlia, C. G. Ang, S. Gossert, A. A. Rashad Ahmed, M. A. Hossain, C. F. Abrams, A. B. Smith III, I. Chaiken (2021). “HIV-1 Env-dependent cell killing by bifunctional small-molecule/peptide conjugates.” *ACS Chem. Biol.* **16**, 193-204. doi:10.1021/acschembio.0c00888 PMID:33410670
116. B. Parajuli, K. Acharya, A. Nangarlia, S. Zhang, B. Parajuli, A. Dick, B. Ngo, C. F. Abrams, I. Chaiken (2020). “Identification of a glycan cluster in gp120 essential for irreversible HIV-1 lytic inactivation by a lectin-based recombinantly engineered protein conjugate.” *Biochem. J.* **477**, 4263-4280. doi:10.1042/BCJ20200495 PMID:33057580
115. S. Gossert, B. Parajuli, I. Chaiken, C. F. Abrams (2020). “Roles of variable linker length in dual acting virucidal entry inhibitors on HIV-1 potency via on-the-fly free energy molecular simulations.” *Protein Sci.* **29**, 2304. doi:10.1002/pro.3949 PMID:32926485

114. S. P. Anand, Y. Chen, J. Prévost, R. Gasser, G. Beaudoin-Bussiéres, C. F. Abrams, M. Pazgier, A. Finzi (2020). “Interaction of human ACE2 to membrane-bound SARS-CoV-1 and SARS-CoV-2 S glycoproteins.” *Viruses* **12**, 1104. doi:10.3390/v12101104 PMID:33003587
113. Jérémie Prévost, William D. Tolbert, Halima Medjahed, Rebekah T. Sherburn, Navid Madani, Daria Zoubchenok, Gabrielle Gendron-Lepage, Althea E. Gaffney, Melissa C. Grenier, Sharon Kirk, Natasha Gupta Vergara, Changze Han, Brendan T. Mann, Agnès L. Chénine, Adel Ahmed, Irwin Chaiken, Frank Kirchhoff, Beatrice H. Hahn, Hillel Haim, **Cameron F. Abrams**, Amos B. Smith, III, Joseph Sodroski, Marzena Pazgier, Andrés Finzi (2020). “The HIV-1 Env gp120 Inner Domain Shapes the Phe43 Cavity and the CD4 Binding Site.” *mBio* **11**, e00280-20. doi:10.1128/mBio.00280-20 PMID:32457241
112. Shitao Zou, Shijian Zhang, Althea Gaffney, Haitao Ding, Maolin Lu, Jonathan Grover, Mark Farrell, Hanh Nguyen, Connie Zhao, Saumya Anang, Meiqing Zhao, Mohammadjavad Mohammadi, Scott Blanchard, Cameron Abrams, Navid Madani, Walther Mothes, John Kappes, Amos Smith, III, Joseph Sodroski (2020). “Long-Acting BMS-378806 Analogues Stabilize the State-1 Conformation of the Human Immunodeficiency Virus (HIV-1) Envelope Glycoproteins.” *J. Virol.* **94**, e00148-20. doi:10.1128/JVI.00148-20 PMID:32161177
111. Charles Ang, Mohammed Hossain, Marg Rajpara, Harry Bach, Kriti Acharya, Alexej Dick, Adel Ahmed, Michelle Kutzler, **Cameron F. Abrams**, Irwin Chaiken (2020). “Metastable HIV-1 Surface Protein Env Sensitizes Cell Membranes to Transformation and Poration by Dual-Acting Virucidal Entry Inhibitors.” *Biochemistry* **59**, 818-828. doi:10.1021/acs.biochem.9b01008 PMID:31942789
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, Amos B. Smith, III (2020). “Optimization of Small Molecules for their Capacity to Sensitize HIV-1 Infected Cells to Antibody Dependent Cellular Cytotoxicity.” *ACS Med. Chem. Lett.* **11**, 371-378. doi:10.1021/acsmedchemlett.9b00445 PMID:32184972
109. Jasmine Gardner, **Cameron F. Abrams** (2019). “Energetics of Flap Opening in HIV-1 Protease: String Method Calculations.” *J. Phys. Chem. B* **123**, 9584-9591. doi:10.1021/acs.jpcb.9b08348 PMID:31640343
108. Anindya Bhaduri, Jasmine Gardner, **Cameron F. Abrams**, Lori Brady (2019). “Free energy calculation using space filled design and weighted reconstruction: A modified single sweep approach.” *Mol. Sim.* **46**, 193-206. doi:10.1080/08927022.2019.1688325 PMID:39780972
107. Shilei Ding, Melissa Grenier, William Tolbert, Dani Vézina, Rebekah Sherburn, Jonathan Richard, Jérémie Prévost, Jean-Philippe Chapleau, Gabrielle Gendron-Lepage, Halima Medjahed, **Cameron F. Abrams**, Joseph Sodroski, Marzena Pazgier, Amos Smith, III, Andrés Finzi (2019). “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. doi:10.1128/JVI.01325-19 PMID:31554684
106. Gourav Shrivastav, Eric Vanden-Eijnden, **Cameron F. Abrams** (2019). “Mapping Saddles and Minima on Free Energy Surfaces using Multiple Climbing Strings.” *J. Chem. Phys.* **151**, 124112. doi:10.1063/1.5120372 PMID:31575198
105. Connie Zhao, Amy Princiotto, Hanh Nguyen, Shitao Zou, Meiqing Zhao, Shijian Zhang, Alon Herschhorn, Mark Farrell, Karanbir Pahil, Bruno Melillo, Somisetti Sambasivarao, Cameron Abrams, Amos Smith III, Navid Madani, Joseph Sodroski (2019). “Strain-dependent activation and inhibition of human immunodeficiency virus (HIV-1) entry by a specific PF-68742 stereoisomer.” *J. Virol.* **93**, 1-20. doi:10.1128/JVI.01197-19 PMID:31391272
104. Ming Huang, **Cameron F. Abrams** (2019). “Effects of Reactivity Ratios on Network Topology and Thermomechanical Properties in Vinyl-Ester/Styrene Thermosets: Molecular Dynamics Simulations.” *Macromol. Theory. Sim.* **28**, 1900030. doi:10.1002/mats.201900030

103. Arun Srikanth Sridhar, **Cameron F. Abrams** (2019). “Effect of molecular packing and hydrogen bonding on the properties of epoxy-amido amine systems.” *Comput. Mater. Sci.* **169**, 109082. doi: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 F. Abrams**, James B. Munro, Adrian B. McDermott, Andrés Finzi, Peter D. Kwong, Scott C. Blanchard, Joseph G. Sodroski, Walther Mothes (2019). “Associating HIV-1 envelope glycoprotein structures with states on virus observed by smFRET.” *Nature* **568**, 415-419. doi:10.1038/s41586-019-1101-y PMID:30971821
101. Arun Srikanth Sridhar, **Cameron F. Abrams** (2019). “Yield and Post-yield Behavior of Fatty-Acid-Functionalized Amidoamine–Epoxy Systems: A Molecular Simulation Study.” *J. Dyn. Behav. Mater.* **5**, 143-149. doi:10.1007/s40870-019-00193-z PMID:39790932
100. Ryan Gordon, Spencer Stober, **Cameron F. Abrams** (2018). “Counterion Effects on Aggregate Structure of 12-Hydroxystearate Salts in Hexane: A Quantum Mechanical and Molecular Dynamics Simulation Study.” *J. Phys. Chem. B* **123**, 534-541. doi:10.1021/acs.jpcb.8b08477 PMID:30571113
99. Jasmine Gardner, **Cameron F. Abrams** (2018). “Lipid flip-flop vs. lateral diffusion in the relaxation of hemifusion diaphragms.” *BBA-Biomembranes* **1860**, 1452-1459. doi:10.1016/j.bbamem.2018.04.007 PMID:29684332
98. Steven Gossert, Bibek Parajuli, Irwin Chaiken, **Cameron F. Abrams** (2018). “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. doi:10.1002/prot.25504 PMID:29633345
97. S. Alexis Paz, Luca Maragliano, **Cameron F. Abrams** (2018). “The effect of intercalated water on potassium ion transport through Kv1.2 channels studied via on-the-fly free-energy parameterization.” *J. Chem. Theory. Comput.* **14**, 2743–2750. doi:10.1021/acs.jctc.8b00024 PMID:29570282
96. Arun Sridhar, John Vergara, Emre Kinaci, Giuseppe Palmese, **Cameron F. Abrams** (2018). “The effect of alkyl chain length on mechanical properties of fatty-acid-functionalized amidoamine-epoxy system.” *Comput. Mater. Sci.* **150**, 70-76. doi:10.1016/j.commatsci.2018.03.073
95. S. Alexis Paz, **Cameron F. Abrams** (2018). “Testing Convergence of Different Free-Energy Methods in a Simple Analytical System with Hidden Barriers.” *Computation* **6**, 27. doi:10.3390/computation6020027
94. Bibek Parajuli, Kriti Acharya, Harry C. Bach, Bijay Parajuli, Shiyu Zhang, Amos B. Smith III, **Cameron F. Abrams**, Irwin Chaiken (2018). “Restricted HIV-1 Env Glycan Engagement by Lectin-Reengineered DAVEI Protein Chimera is Sufficient for Lytic Inactivation of the Virus.” *Biochem. J.* **475**, 931-957. doi:10.1042/BCJ20170662 PMID:29343613
93. Francesca Moraca, David Rinaldo, Amos B. Smith, III, **Cameron F. Abrams** (2018). “Specific Non-Covalent Interactions Determine Optimal Structure of a Buried Ligand Moiety: QM/MM and Pure QM Modeling of Complexes of the Small-Molecule CD4 Mimetics and HIV-1 Gp120.” *ChemMedChem* **13**, 627-633. doi:10.1002/cmdc.201700728 PMID:29337418
92. Jasmine Gardner, **Cameron F. Abrams** (2017). “Rate of hemifusion diaphragm dissipation and ability to form three-junction bound HD determined by lipid composition.” *J. Chem. Phys.* **147**, 134903. doi:10.1063/1.4994320 PMID:28987088
91. Ryan Gordon, Spencer Stober, **Cameron F. Abrams** (2017). “Effects of Optical Purity and Finite System Size on Self-Assembly of 12-Hydroxystearic Acid in Hexane: Molecular

Dynamics Simulations." *J. Phys. Chem. B* **121**, 9223-9233. doi:10.1021/acs.jpcb.7b05246 PMID:28876930

90. Alon Herschhorn, Christopher Gu, Francesca Moraca, Xiaochu Ma, Mark Farrell, Amos B. Smith, III, Marie Pancera, Peter D. Kwong, Arne Schön, Ernesto Freire, Cameron Abrams, Scott C. Blanchard, Walther Mothes, Joseph G. Sodroski (2017). "The β20-β21 of gp120 is a regulatory switch for HIV-1 Env." *Nature Comm.* **8**, 1049. doi:10.1038/s41467-017-01119-w PMID:29051495
89. Kriti Acharya, Adel A. Rashad, Francesca Moraca, Per Johan Klasse, John P. Moore, **Cameron F. Abrams**, Irwin Chaiken (2017). "Recognition of HIV-Inactivating Peptide Triazoles by a Recombinant Soluble Trimer, BG505 SOSIP.664." *Proteins* **85**, 843-851. doi:10.1002/prot.25238 PMID:28056499
88. Arun Sridhar, John Vergara, Giuseppe Palmese, **Cameron F. Abrams** (2017). "The Effect of Alkyl Chain Length on Material Properties of Fatty-Acid-Functionalized Amidoamine-Epoxy Systems." *Eur. Polymer J.* **89**, 1-12. doi:10.1016/j.eurpolymj.2017.01.037
87. Jungho Yang, Arun Srikanth, Changwoon Jang, **Cameron F. Abrams** (2017). "Relationships Between Molecular Structure and Thermomechanical Properties of Bio-Based Thermosetting Polymers." *J. Polym. Sci. B Pol. Phys.* **55**, 285-292. doi:10.1002/polb.24270
86. S. Alexis Paz, Eric Vanden-Eijnden, **Cameron F. Abrams** (2017). "Polymorphism at 129 Dictates Metastable Conformations of the Human Prion Protein N-terminal β-sheet." *Chem. Sci.* **8**, 1225-1232. doi:10.1039/C6SC03275C PMID:28451263
85. Bibek Parajuli, Kriti Acharya, Reina Yu, Adel A. Rashad, **Cameron F. Abrams**, Irwin M. Chaiken (2016). "Lytic Inactivation of HIV-1 by Dual Engagement of gp120 and gp41 Domains in the Virus Env Trimer." *Biochemistry* **55**, 6100-6114. doi:10.1021/acs.biochem.6b00570 PMID:27731975
84. Francesca Moraca, Kriti Acharya, Bruno Melillo, Amos B. Smith, III, Irwin M. Chaiken, **Cameron F. Abrams** (2016). "Computational Evaluation of HIV-1 gp120 Conformations of Soluble Trimeric gp140 Structures as Targets for de novo Docking of First- and Second-Generation Small-Molecule CD4 Mimetics." *J. Chem. Info. Model.* **56**, 2069-2079. doi:10.1021/acs.jcim.6b00393 PMID:27602436
83. Tang-Qing Yu, Jianfeng Lu, **Cameron F. Abrams**, Eric Vanden-Eijnden (2016). "A Multiscale Implementation of Infinite-Swap Replica Exchange Molecular Dynamics." *Proc. Natl. Acad. Sci. USA* **113**, 11744-11749. doi:10.1073/pnas.1605089113 PMID:27698148
82. Changwoon Jang, **Cameron F. Abrams** (2016). "Thermal and Mechanical Properties of Thermosetting Polymers using Coarse-grained Simulation." *Eur. Phys. J. Spec. Top.* **225**, 1775-1783. doi:10.1140/epjst/e2016-60143-0 PMID:27627411
81. Ryan Gordon, Spencer S. Stober, **Cameron F. Abrams** (2016). "Aggregation of 12-Hydroxystearic Acid and Its Lithium Salt in Hexane: Molecular Dynamics Simulations." *J. Phys. Chem. B.* **120**, 7164-7173. doi:10.1021/acs.jpcb.6b04193 PMID:27387154
80. Jasmine Gardner, Markus Deserno, **Cameron F. Abrams** (2016). "Effect of Intrinsic Curvature and Edge Tension on the Stability of Binary Mixed-Membrane Three-Junctions." *J. Chem. Phys.* **145**, 074901. doi:10.1063/1.4960433 PMID:27544120
79. Anthony Bucci, Tang-Qing Yu, Eric Vanden-Eijnden, **Cameron F. Abrams** (2016). "Kinetics of O2 Entry and Exit in Monomeric Sarcosine Oxidase via Markovian Milestoning Molecular Dynamics." *J. Chem. Theory Comput.* **12**, 2964-2972. doi:10.1021/acs.jctc.6b00071 PMID:27168219
78. Changwoon Jang, Majid Sharifi, Giuseppe Palmese, **Cameron F. Abrams** (2016). "Toughness enhancement of thermosetting polymers using a novel partially reacted substructure curing protocol: A combined molecular simulation and experimental study." *Polymer* **90**, 249-255. doi:10.1016/j.polymer.2016.03.023 PMID:39790414

77. Ramalingam Venkat Kalyana Sundaram, Huiyuan Li, Lauren Bailey, Adel A. Rashad, Rachna Aneja, Karl Weiss, James Huynh, Arangaserry Rosemary Bastian, Elisabeth Papazoglou, Cameron Abrams, Steven Wrenn, Irwin Chaiken (2016). "Impact of HIV-1 Membrane Cholesterol on Cell-Independent Lytic Inactivation and Cellular Infectivity." *Biochemistry* **55**, 447-458. doi:10.1021/acs.biochem.5b00936 PMID:26713837
76. Majid Sharifi, Changwoon Jang, **Cameron F. Abrams**, Giuseppe Palmese (2015). "Epoxy Polymer Networks with Improved Thermal and Mechanical Properties via Controlled Dispersion of Reactive Toughening Agents." *Macromolecules* **48**, 7495-7502. doi:10.1021/acs.macromol.5b00677
75. S. Alexis Paz, **Cameron F. Abrams** (2015). "Free Energy and Hidden Barriers of the β-Sheet Structure of Prion Protein." *J. Chem. Theory Comput.* **11**, 5024-5034. doi:10.1021/acs.jctc.5b00576 PMID:26574287
74. Tang-Qing Yu, Mauro Lapelosa, Eric Vanden-Eijnden, **Cameron F. Abrams** (2015). "Full kinetics of CO entry, internal diffusion, and exit in myoglobin from transition-path theory simulations." *J. Amer. Chem. Soc.* **137**, 3041-3050. doi:10.1021/ja512484q PMID:25664858
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1. Yaping Zhong, **Cameron F. Abrams**, P. K. Lim. (1995). “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. doi:10.1021/ie00044a003 PMID:39744149

## SEMINARS AND PRESENTATIONS

### *Invited Seminars*

67. “Molecular Simulations of Thermosetting Polymers,” North Carolina State University, Dept. of Chemical and Biomolecular Engineering, 3 April 2026.
66. “Molecular Simulations of Thermosetting Polymers,” University of Virginia, Dept. of Chemical Engineering, 2 October 2024.
65. “Modern Molecular Simulations Using Extended Lagrangian Approaches,” National Institute of Chemistry, Slovenia, 18 June 2024.

64. “Modern Molecular Simulations Using Extended Lagrangian Approaches,” National University of Cordoba, Argentina, Department of Chemistry, 25 March 2024.
63. “Molecular Simulations of Thermosetting Polymers,” Northeastern University, Dept. of Chemical Engineering, 5 December 2023.
62. “Molecular Simulations of Thermosetting Polymers,” Lehigh University, Dept. of Chemical and Biomolecular Engineering, 9 November 2022.
61. “Recent simulation methods for resolving molecular details in thermodynamics and kinetics,” University of South Florida, Dept. of Chemical Engineering, 3 March 2021 (via Teams).
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, .
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, .
7. “Inhomogeneous Coarse-Graining of Polymers and Polymer/Metal Interfaces,” FZ Jülich Workshop on Computational Soft Matter, Bonn, Germany, .
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, .
4. “Comparison of Coarse-Graining Schemes for Structural Investigation of Polycarbonate Liquids via Simulation,” Division of Engineering and Applied Science, California Institute of Technology, .
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, .
1. “Molecular Dynamics Simulations of Reactive Ion Bombardment of Silicon Surfaces,” Ph.D. Colloquium, Department of Chemical Engineering, University of California, Berkeley, .

***Contributed Presentations***

83. Gourav Shrivastav, Eric Vanden-Eijnden, and **Cameron F. Abrams**, “Mapping Saddles and Minima on Free Energy Surfaces Using Multiple Climbing Strings,” Annual Meeting of the American Institute of Chemical Engineers, Orlando, Florida, 11 November 2019.
82. Ming Huang and **Cameron F. Abrams**, “Interrelating Relative Reactivity, Network Topologies, and Thermochemical Properties in Vinyl-Ester Thermosets Using All-Atom Molecular Simulations,” Annual Meeting of the American Institute of Chemical Engineers, Orlando, Florida, 12 November 2019.
81. Salman Zarrini and **Cameron F. Abrams**, “Multi-scale Modeling of Fiber-Matrix Interphase,” Annual Meeting of the American Institute of Chemical Engineers, Orlando, Florida, 11 November 2019.
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 β-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, Giuseppe 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-triazole dual-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 $\alpha$1 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, , 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, , 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, , 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, , 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, , 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 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 SiO2 Surfaces: Molecular Dynamics Simulations," 44th International Symposium of the American Vacuum Society, , 20-24 October 1998.

## FUNDED PROPOSALS

***Research Grants***

24. **"Combining Molecular Simulations and Biophysical Methods to Characterize Conformational Dynamics of the HIV-1 Envelope Glycoprotein"** — NIH , R01 AI178833 , $4,091,232 7/10/2023-6/30/2028
    Co-PIs: Joe Sodroski, Dana Farber Cancer Institute/Harvard Medical School; Walther Mothes, Yale
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 9/1/17-5/31/21
    Co-I: Eric Vanden-Eijnden, NYU
22. **"Thermosets for Agile Manufacturing,"** — Army Research Lab , W911NF-17-2-0227 , $3,000,000 9/1/17-12/31/23
    Co-I (PI: G. R. Palmese)
21. **"Biobased Thermosetting Polymers for Composite, Adhesive, and Coating Applications,"** — Army Research Lab , W911NF-12-R-0011 , $2,400,000 1/1/17-12/31/19
    Co-I (PI: G. R. Palmese) Abrams' share supported one FTE PhD student.
20. **"Dual-action virolytic entry inhibitors against HIV-1"** — NIH , R01 GM115249 , 1,700,000 7/1/15-6/30/19
    Multiple-PI grant; other Co-PI is Irwin Chaiken, DUCOM. Abrams' share supports one FTE PhD student.
19. **"Structure-based antagonism of HIV-1 envelope function in cell entry"** — NIH , $10,000,000 9/30/13-8/31/23
    Co-I (PI: I. Chaiken) 9/30/13-8/31/23. Abrams is the leader of the Computational Core of this program project, directly supervising one postdoc and an annual direct cost of $136,000.
18. **"Drexel/ExxonMobil Sponsored Research Agreement: Advanced Studies of Self-Assembly"** — ExxonMobil , $460,000 1/1/14-12/31/17

17. **"Center for Sustainable Corrosion Protection"** — Army Research Lab , W911NF-13-2-0046 , $3,000,000 9/1/13-8/31/18
    Co-I (PI: G. R. Palmese)
16. **"Collaborative Research: Multiscale molecular simulations of protein-mediated bilayer fusion,"** — NSF , MCB-1330205 , $350,000 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 , DMR-1207389' , $286,455 9/1/12-8/31/15
    NYU (Vanden-Eijnden) is the secondary institution, receiving about the same amount.
14. **"Materials in Extreme Dynamic Environments: The Johns Hopkins Consortium"** — Army Research Lab (through U. Del./JHU) , $300,000 4/2012-3/2020
    (PI: KT Ramesh, JHU)
13. **"Approaches to computing diffusion rates in proteins from transition path theory"** — NIH , R01 GM100472 , $1,100,000 9/1/11-5/31/16
    (Co-I: Eric Vanden-Eijnden, NYU)
12. **"PASI: Molecular-Based Multiscale Modeling and Simulation; Montevideo, Uruguay; September 1-14, 2012"** — NSF , OISE-1124480' , $100,000 9/2024
    (PI: Jim Pfaendtner, UW)
11. **"HIV-1 gp120 conformational transitions in activation and antagonism"** — NIH , R21 AI093248 , $450,000 4/1/11-3/31/13
    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' , $55,000 1/1/11-12/31/11
    (Co-I: Mike White, DUCOM Biochemistry)
9. **"MRI: Acquisition of a GPU-Accelerated High Performance Computing Cluster"** — NSF , AST-0959884 , $440,000 3/1/10-2/28/11
8. **"Chimeric Virucides Based on a Novel Theory of Viral Metastability"** — NIH , R01 AI084117 , $1,300,000 9/1/09-8/31/13
    (Co-I Irwin Chaiken, DUCOM Biochemistry)
7. **"DURIP: Acquisition of a High-Performance Computer Cluster"** — Army Research Lab , W911NF-07-1-0301 , $120,000 6/15/07-6/14/08
6. **"Drexel-ARL Materials Center of Excellence in Polymeric Materials"** — Army Research Lab , W911NF-06-2-0013 , $1,350,000 3/30/2006-3/31/2011
    (PI: Giuseppe Palmese; Co-Is Yossef Elabd and Chris Li)
5. **"CAREER: Multiscale simulation of solute transport in hydrogels"** — NSF , CBET-0544933 , $400,000 2/1/2006-1/31/2010
4. **"Thermodynamics of Heteropolymers in Confinement"** — American Chemical Society , PRF 42368-G7 , $35,000 2/2005-1/2007
3. **"ITR: Inhomogeneously Resolved Simulation of Protein Assembly Dynamics"** — NSF , DMR-0427643 , $420,000 9/2004-8/2008
2. **"ONR-YIP: Predicting Failure in Carbon Nanotube Reinforced Polymer Composites: A Novel Multiscale Simulation Approach"** — Office of Naval Research , N00014-03-1-0655' , $332,313 6/2003-5/2006
1. **"QSB: Quantitative Simulation of Cell Migration in Porous Biomaterials"** — NSF , CBET-0331191' , $96,129 11/2003-10/2005

***Supercomputer Allocations***

3. **"Molecular Dynamics Studies of Epoxies,"** — DoD HPCMP , 9M hours through 10/31/2024
2. **"Molecular Dynamics Studies of Various Protein Systems"** — NSF ACCESS , MCB080073N 7/1/2007-present
1. **"Molecular Simulation of Mechanical Deformation of Filled Epoxies"** — NSF TeraGrid , 30,000 hours 9/1/2006-9/1/2007

***Pending / Planned***

1. **"New CD4 mimetics targeting conformational vulnerabilities of the HIV-1 envelope glycoprotein"** — NIH , $700,00
(MPI: Co-PIs's Andrés Finzi (UMontreal) and Amos Smith III (UPenn))

## PATENTS

"Recombinant Chimeric Cyanovirin-MPER Constructs for Inactivating HIV-1," US Patent #10,603,545 B2. March 31, 2020
Inventors: Irwin M. Chaiken, Cameron F. Abrams, Mark A. Contarino, Arangassery R. Bastian

## STUDENTS AND POSTDOCS SUPERVISED

***Ph.D.***

19. **Prince Gyasi**, "MD Simulations of HIV-1 Env" — Dates of supervision: 9/24-. Supported by NIH R01 AI178833.
18. **Imran Yasin**, "Molecular Simulations of Thermoset Additive Manufacturing" — Dates of supervision: 3/20-3/21. Supported by W911NF-17-2-0227. Left PhD program.
17. **Dr. Ming Huang**, "Molecular Simulations of Thermoset Additive Manufacturing" — Dates of supervision: 11/17-8/22. Supported by W911NF-17-2-0227.
16. **Matthew Cameron**, "Milestoning MD of Ligand Binding Kinetics" — Dates of supervision: 11/16-8/17. Left PhD program.
15. **Donald Seaman**, "Molecular Simulations of Bio-based Thermosets" — Dates of supervision: 11/16-6/19. Left PhD program. Supported by W911NF-12-R-0011.
14. **Dr. Natasha Vergara**, "Computational Design of HIV-1 Entry Inhibitors" — Dates of supervision: 11/16-8/22. Currently at Bristol-Myers-Squibb.
13. **Dr. Steven Gossert**, "Novel HIV-1 Virucides" — Dates of supervision: 11/15-6/20. Supported on NIH GM115249. Currently at Bristol-Myers-Squibb.
12. **Dr. Jasmine Gardner**, "Lipid and protein contributions to viral proliferation as studied using MD simulations and advanced MD techniques" — Dates of supervision: 11/14-6/19. Supported on NSF MCB-1330205. Now a Postdoc at Uppsala University
11. **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
10. **Dr. Ryan Gordon**, "Molecular Simulation Studies Self-Assembly" — Dates of Supervision: 11/13-06/18. Supported on ExxonMobil SRA. Now at Lockheed Martin.
9. **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.
8. **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.
7. **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
6. **Dr. Spencer Stober**, "Protein Conformational Changes" — Dates of supervision: 1/08-9/12. Support: Part-time PhD
5. **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.

4. **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 a full professor in the Chemical Engineering Department and the University of New Hampshire."
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)
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

***Postdoctoral***

12. ***Dr. Salsabil Abou-Hatab**, "MD Simulations of HIV-1 Env" — 2023-. Supported by NIH R01 AI178833.
11. **Dr. Ketan Khare**, "Dynamics of Thermosetting Polymers" — 2020-2021. Supported by W911NF-17-2-0227.
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: 2018-2022. Supported on NIH R01 GM 100472.
8. **Dr. Salman Zarrini**, "Molecular Simulation Studies of Thermosets" — Dates of supervision: 2018-2022. Supported W911NF-13-2-0046 and W911NF-17-2-0227.
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.
5. **Dr. Francesca Moraca**, "Computational Drug Design of HIV-1 Entry Inhibitors" — Dates of supervision: 2014-2016. Supported on NIH P01 GM056550. Currently employed at Schrodinger
4. **Dr. Sergio Alexis Paz**, "On-the-fly free energy parameterization" — Dates of supervision: 2014-2016. Supported on NSF DMR-1207389. Currently an associate 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.
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 research associate at University of British Columbia.

***Masters***

2. ***Matthew Gilpin. "Studies of Protein Conformational Dynamics"**, "Dates of supervision: 7/21-."
1. **Shyno Mathew. "Studies of O2 diffusion in monomeric sarcosine oxidase"**, "Dates of supervision: 6/08-6/10. Graduated BS/MS June 2010."

***Undergraduate***

17. **Megan Gatchel (REU)**, "SARS-CoV-2 Variants Studied using Molecular Simulations" — 2021.
16. **Theodore Houser**, "Classification of HIV-1 Entry Inhibitors" — 2021.
15. **Marta Martinez**, "Classification of HIV-1 Spike Glycoprotein Structures" — 2020-2021.

14. **Nicholas Carpentieri**, “Classification of HIV-1 Entry Inhibitors” — 2020-2021.
13. **Noor Al-Nazal**, “Thermoset Molecular Simulations” — 2020.
12. **Ian O’Donnell**, “Cheminformatics Website and Database in PHP/MariaDB” — 2020-2021.
11. **Zach Lloyd (REU)**, “Molecular Simulations in Thermoset Materials” — 2020.
10. **Ai Vi Truong**, “Molecular Simulations in Thermoset Materials” — 2020.
9. **Yen La**, “Molecular Simulations in Thermoset Materials” — 2020.
8. **Ariel Yeung**, “Molecular Simulations in HIV” — 2019.
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
3. **Charles Bender**, “2-D Wang-Landau Monte Carlo” — Summer STAR
2. **Christopher Petersen**, “2-D Wang-Landau Monte Carlo” — Summer STAR
1. **Suroor Manzoor**, “Bitwise Voxelized 3D Domains: Toward Efficient Simulation of Diffusion in Porous Media” — 2/2003-7/2003.

## HONORS & AWARDS

Inaugural Bartlett ’81 – Barry ’81 Professor of Chemical and Biological Engineering — *Drexel University* 2022
Provost Award for Outstanding Career Scholarly Achievement — *Drexel University* 2020
College of Engineering Outstanding Career Research Award — *Drexel University* 2020
Department of Chemical and Biological Engineering Research Award — *Drexel University* 2017
Impact Award in Computational Molecular Science and Engineering — *American Institute of Chemical Engineers* 2015
Fellow — *American Institute of Medical and Biological Engineering* 2015
College of Engineering Research Award — *Drexel University* 2014
Invited Participant, “Physical Principles of Multiscale Modeling, Analysis and Simulation in Soft Condensed Matter,” — *Kavli Institute for Theoretical Physics, UCSB* 2012
General Participant, “German-American Frontiers of Engineering” Symposium — *National Academy of Engineering* 2008
Graduate Mentor of the Year — *Drexel University* 2007
CAREER Awardee — *NSF* 2006
General Participant, “Frontiers of Engineering” Symposium — *National Academy of Engineering* 2004
Young Investigator Awardee — *Office of Naval Research* 2006
Chevron Graduate Fellow — *University of California, Berkeley, Dept. Chem. Engr.* 1998
2nd Place, Poster Competition, N — *Northern California AVS Thin Films User Group* 1997
1st Place, Southern Regional Undergraduate Paper Contest — *American Institute of Chemical Engineers* 1995
3rd Place, Southern Regional Undergraduate Paper Contest — *American Institute of Chemical Engineers* 1994
Phi Kappa Phi Inductee — *NCSU* 1991
Eastman Scholar — *NCSU* 1991

## SERVICE

***Department of Chemical and Biological Engineering, Drexel University***

- Chair, Graduate Committee, 2008-2014 (Member 2008-present)
- Member, Undergraduate Committee, 2008-present
- Member, Committee on Academic Standing, 2008-2017; Chair, 2014-2017

- Graduate Advisor, 2008-2014
- Standing Member, Faculty Search Committee
- Standing Member, Faculty Evaluation Committee
- Faculty Advisor, AIChE Student Chapter, 2004-2006
- Seminar series organizer, 2003-2006
- Department Head, 2017-

***College of Engineering, Drexel University***

- Member, Junior Advisory Committee, 2006-2008
- Member, Senior Advisory Committee, 2008-2010
- Member, Tenure and Promotion Committee, 2015-2017
- Member, Task Force on Computational Engineering Minor, 2015-2016
- Chair, Electrical and Computer Engineering Department Head Search Committee, 2018
- Chair, Materials Science and Engineering Department Head Review Committee, 2019

***University***

- Workshop tutor, Drexel Center for Academic Excellence, 2002-2003
- Scholars Day Interviewer, 2003 & 2005
- Open Houses (several)
- Member of the Faculty Senate representing COE, 2010-2013
- Member, COE Dean's Search Committee, 2010-2011 (Search failed)
- Member, Senate Committee on Research and Scholarly Activities, 2010-2013. Chair, 2011-2013
- Member, Strategic Initiative #4 Implementation Task Force, 2012-2013
- Member, Computing Task Force, 2012-2013
- Chair, Board of Governance of the University Research Computing Facility, 2013-2017
- Member, Lebow College of Business Dean's Search Committee, 2012-2014; Hired Frank Linnehan
- Member, CIO Search Committee, 2015; Hired Tom DiChiaro.
- Provost's Fellow, CY 2016, under SVPR Aleister Saunders.
- Member, Review Committee for CoE Dean Joseph Hughes, 2016
- Member, Return to Campus Oversight Committee, 2020-2022

***Profession***

- National member: AIChE, ACS, AIMBE
- Session Chair, AIChE Annual Meetings, 2004-2011
- Session Chair, ACS Annual Meeting, 2016
- Session Co-organizer, APS March Meeting, 2004
- Session Organizer, APS March Meeting, 2005:
- "Theory and Simulation of Polymers I: General"
- "Theory and Simulation of Polymers II: Surfaces and Confinement"
- Ad-hoc Proposal Reviewer (counts): NSF (18), ACS (4), NIH (3), ESF (2), DTRA (1), AVH (1), ISF (1)
- Review Panelist (counts): NSF (9), NIH (12)
- Site visit panel: NSF-STC (1, Chair)
- Referee for the following journals (counts as of June 2024; 236 total):

## COURSES DEVELOPED

4. **CHE 800-002: Molecular Simulation (2003-04 Spring Term, 2020-21 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, metadynamics) were all covered in this course. Extensive course web pages were developed and continue to be maintained as a reference (). Students were evaluated based on individual term projects.
3. **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.
2. **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.

1. **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. Abrams led instruction in the next academic year.

## SOFTWARE

**Pestifer** — A builder for all-atom molecular simulations of biological molecules
**Ycleptic** — A utility for specifying and parsing configuration input files in YAML
**Pidibble** — A PDB file parser
**HTPolyNet** — A builder for all-atom molecular simulation systems of dense crosslinked polymers
**CFACV** — A collective-variables module for NAMD2 (available at github/cameronabrams)