Justin A. Lemkul, Ph.D. — Associate Professor of Biochemistry

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Education

2012 **Ph.D., Biochemistry**
Virginia Polytechnic Institute and State University
MILES-IGERT Graduate Certificate

2007 **B.S. In Honors, Biochemistry (Summa Cum Laude)**
Virginia Polytechnic Institute and State University
Minor in Chemistry, Concentration in Biotechnology

Employment and Experience

2023 – Present **Associate Professor**
Department of Biochemistry, Virginia Polytechnic Institute and State University

2017 – 2023 **Assistant Professor**
Department of Biochemistry, Virginia Polytechnic Institute and State University

2013 – 2017 **NIH Ruth L. Kirschstein Postdoctoral Fellow**
Department of Pharmaceutical Sciences and Computer-Aided Drug Design Center, University of Maryland, Baltimore

2012 – 2013 **Research Scientist**
Department of Biochemistry, Virginia Polytechnic Institute and State University

2007 – 2012 **Graduate Research Assistant**
Department of Biochemistry, Virginia Polytechnic Institute and State University

Awards and Honors

2025 College of Agriculture & Life Sciences Outstanding Graduate Student Mentor
2024 Department of Biochemistry Service and Outreach Award
2023 Virginia Tech Graduate School Mentor of the Month (May)
2022 Department of Biochemistry Research Award
2022 OpenEye Outstanding Junior Faculty Award (American Chemical Society COMP Division)
2021 Department of Biochemistry Teaching Award
2017 1st Place poster (Pharmaceutical Sciences postdoc category), UMB School of Pharmacy Research Day
2016 The Wiley Computers in Chemistry Outstanding Postdoc Award (American Chemical Society COMP Division)
2013 Virginia Tech Graduate School Outstanding Dissertation in Science, Technology, Engineering, and Mathematics
2012 Virginia Tech College of Agriculture and Life Sciences Outstanding Doctoral Student
2011 Kendall W. King Memorial Scholarship (outstanding senior Biochemistry graduate student)
2009 1st Place poster (Student Biomedical category), 6th Annual VCOM Research Day

2009	James F. Eheart Travel scholarship
2008	Bruce M. Anderson Graduate Award (outstanding first-year Biochemistry graduate student)
2008 – 2010	NSF MILES-IGERT Training Grant for Research in Oxidative Processes
2007 – 2012	Institute for Critical Technology and Applied Science (ICTAS) Doctoral Scholar Graduate Fellowship
2007	James Lewis Howe Award (Blue Ridge Chapter of the American Chemical Society)
2006	Phi Beta Kappa National Arts and Sciences Honor Fraternity
2005, 2006	R. W. Engel Scholarship
2003 – 2007	Dean's List

Professional Memberships and Service

2024 – 2026	Executive Council Member, Biophysical Society Theory & Computation Subgroup
2020 – Present	Sigma Xi (Full Member)
2020 – Present	Virginia Academy of Science
2014 – Present	Biophysical Society
2010 – Present	American Chemical Society
2006 – Present	Phi Beta Kappa National Arts and Sciences Honor Fraternity (Junior-year inductee)
2004 – Present	Alpha Chi Sigma Professional Chemistry Fraternity

Academic Affiliations

2023 – Present	Affiliate Faculty, Genetics, Bioinformatics, and Computational Biology Program
2023 – Present	Affiliate Faculty, Department of Biological Sciences
2019 – Present	Affiliate Faculty, Division of Systems Biology
2018 – Present	Affiliate Faculty, Center for Drug Discovery

University Service

2024 – 2025	Associate Vice Provost of Faculty Affairs Search Committee
2024 – 2025	Operations Officer, Virginia Tech Faculty Senate
2024 – 2025	Virginia Tech University Council Cabinet
2024 – 2025	Virginia Tech University Council
2023 – 2025	Chair, Virginia Tech Commission on Faculty Affairs
2023 – Present	Virginia Tech Faculty Senate Cabinet
2023 – 2024	Virginia Tech Faculty Senate Policy and Procedures Committee
2022 – 2025	Virginia Tech Commission on Faculty Affairs
2020 – 2026	Faculty Senator, Biochemistry
2018 – 2023	Chapter Advisor, Gamma Iota Chapter of the Alpha Chi Sigma Fraternity

Departmental Service

2024 – 2025	Assistant Professor Search Committee (Macromolecular Complexes)
2023 – 2026	Promotion & Tenure Committee
2023 – Present	Biochemistry Graduate Program Director and Chair, Graduate Program Committee
2022 – 2023	Awards Committee
2022	Communications Committee
2022 – 2023	Department Head Search Committee
2021 – 2022	Assistant Professor Search Committee (Nucleic Acids)
2021 – 2022	Space Committee
2021 – 2022	Promotion & Tenure Committee (non-voting)
2017 – Present	Graduate Program Committee

PEER-REVIEWED PUBLICATIONS (*Corresponding author)

Since starting at Virginia Tech

1. M.D. Polêto and **J.A. Lemkul*** (2025) "Structural and Electronic Properties of Polyethylene Terepththalate (PET) from Polarizable Molecular Dynamics Simulations" *Macromolecules.* 58 (1): 403-414. (Cover Art) (PMC11741139)

2. Y. Nan, P. Baral, A. Orr, H.M. Michel, **J.A. Lemkul**, and A.D. MacKerell, Jr. (2024) "Balancing Group 1 Monoatomic Ion-Polar Compound Interactions in the Polarizable Drude Force Field: Application in Protein and Nucleic Acid Systems" *J. Phys. Chem. B*. 128 (49): 12078-12091. (NIHMS2040473)

3. W. Hwang, S.L. Austin, A. Blondel, E.D. Boittier, S. Boresch, M. Buck, J. Buckner, A. Caflisch, H.-T. Chang, X. Cheng, Y.K. Choi, J.-W. Chu, M. Crowley, Q. Cui, A. Damjanovic, Y. Deng, M. Devereux, X. Ding, M. Feig, J. Gao, D.R. Glowacki, J.E. Gonzales II, M.B. Hamaneh, E. Harder, R.L. Hayes, J. Huang, Y. Huang, P. Hudson, W. Im, S.M. Islam, W. Jiang, M.R. Jones, S. Käser, F.L. Kearns, N.R. Kern, J.B. Klauda, T. Lazaridis, J. Lee, **J.A. Lemkul**, X. Liu, Y. Luo, A.D. MacKerell Jr., D.T. Major, M. Meuwly, K. Nam, L. Nilsson, V. Ovchinnikov, E. Paci, S. Park, R.W. Pastor, C.B. Post, S. Prasad, J. Pu, Y. Qi, T. Rathinavelan, D.R. Roe, B. Roux, C.N. Rowley, J. Shen, A.C. Simmonett, A.J. Sodt, K. Töpher, M. Upadhyay, A. van der Vaart, L.I. Vazquez-Salazar, R.M. Venable, H.L. Woodcock, Y. Wu, C.L. Brooks III, B.R. Brooks, and M. Karplus. (2024) "CHARMM at 45: Enhancements in accessibility, functionality, and speed" *J. Phys. Chem. B.* 128 (41): 9976-10042. (Cover art for Virtual Special Issue: "Recent Advances in Simulation Software and Force Fields") (PMC11492285)

4. **J.A. Lemkul*** (2024) "Introductory Tutorials for Simulating Protein Dynamics with GROMACS" *J. Phys. Chem. B.* 128 (39): 9418-9435. (PMC11457149)

5. J.M. Montgomery and **J.A. Lemkul*** (2024) "Quantifying Induced Dipole Effects in Small Molecule Permeation in a Model Phospholipid Bilayer" *J. Phys. Chem. B.* 128 (30): 7385-7400. (PMC11301690)

6. M.D. Polêto, K.D. Allen,* and **J.A. Lemkul*** (2024) "Structural dynamics of the methyl-coenzyme M reductase active site are influenced by coenzyme F_{430} modifications" *Biochemistry* 63 (14): 1783-1794. (PMC11256747)

7. H.M. Michel and **J.A. Lemkul*** (2024) "Base pair dynamics, electrostatics, and thermodynamics at the *LTR-III* quadruplex:duplex junction" *Biophys. J.* 123 (9): 1129-1138. (PMC11079942)

8. D.S. Davidson and **J.A. Lemkul*** (2024) "Pyroglutamylation Modulates Electronic Properties and the Conformational Ensemble of the Amyloid β-Peptide." *Proteins: Struct, Funct & Bioinf*. 92 (7): 842-853. (PMC11147713)

9. M.D. Polêto and **J.A. Lemkul*** (2023) "Differences in Conformational Sampling and Intrinsic Electric Fields Drive Ion Binding in Telomeric and TERRA G-Quadruplexes." *J. Chem. Inf. Model.* 63 (21): 6851-6862. (PMC10841373)

10. A.F. Wacha and **J.A. Lemkul** (2023) "charmm2gmx: An Automated Method to Port the CHARMM Additive Force Field to GROMACS." *J. Chem. Inf. Model.* 63 (14): 4246-4252. (PMC10369483)

11. N. Giacon, E. Lo Cascio, D.S. Davidson, M.D. Polêto, **J.A. Lemkul**, V. Pennacchietti, L. Pagano, C. Zamparelli, A. Toto, and A. Arcovito (2023) "Structural and functional insights on the interaction between SARS-CoV-2 E protein and ZO1-PDZ2." *Comput. Struct. Biotechnol. J.* 21: 3259-3271. (PMC10210826)

12. B. Grupp, **J.A. Lemkul**, and T. Gronemeyer (2023) "An *in silico* approach to determine inter-subunit affinities in human septin complexes." *Cytoskeleton* 80 (7-8): 141-152. (Special Issue: Molecular and Cell Biology of Septins)

13. D.S. Davidson, J.A. Kraus, J.M. Montgomery, and **J.A. Lemkul*** (2022) "Effects of Familial Alzheimer's Disease Mutations on the Folding Free Energy and Dipole-Dipole Interactions of the Amyloid β-Peptide" *J. Phys. Chem. B* 126 (39): 7552-7566. (PMC9547858)

14. A.M. Salsbury, H.M. Michel, and **J.A. Lemkul*** (2022) "Ion-Dependent Conformational Plasticity of Telomeric G-Hairpins and G-Quadruplexes." *ACS Omega.* 7 (27): 23368-23379. (PMC9280957)

15. A.N. Corrigan and **J.A. Lemkul*** (2022) "Electronic Polarization at the Interface Between the p53 Transactivation Domain and Two Binding Partners" *J. Phys. Chem. B* 126 (26): 4814-4827. (PMC9267131) (Selected for Virtual Special Issue on Biomolecular Electrostatic Phenomena)

16. K.M. King, A.K. Sharp, D.S. Davidson, A.M. Brown,* and **J.A. Lemkul*** (2022) "Impact of Electronic Polarization on Preformed, β-Sheet Rich Homogenous and Heterogeneous Amyloid Oligomers" *J. Comput. Biophys. Chem.* 21 (4): 449-460. (PMC9216210) (Cover art for special issue on Polarizable Force Fields for Biomolecular Modeling)

17. M.D. Polêto and **J.A. Lemkul*** (2022) "TUPÃ: Electric field analyses for molecular simulations" *J. Comput. Chem.* 43 (16): 1113-1119. (PMC9098685)

18. M.D. Polêto and **J.A. Lemkul*** (2022) "Integration of Experimental Data and Use of Automated Fitting Methods in Developing Protein Force Fields" *Commun. Chem.* 5: 38. (PMC8979544) (2022 Editors' Highlights Collection)

19. A.A. Kognole, J. Lee, S.-J. Park, S. Jo, P. Chatterjee, **J.A. Lemkul**, J. Huang, A.D. MacKerell Jr., and W. Im (2022) "CHARMM-GUI Drude Prepper for Molecular Dynamics Simulation Using the Classical Drude Polarizable Force Field" *J. Comput. Chem.* 43 (5): 359-375. (PMC8741736)

20. A.M. Salsbury and **J.A. Lemkul*** (2021) "Monovalent Cation Recruitment and Competition around the *c-kit1* G-Quadruplex Using Polarizable Simulations." *Biophys. J.* 120 (11): 2249-2261. (PMC8390831)

21. A.M. Salsbury and **J.A. Lemkul*** (2021) "Recent Developments in Empirical Atomistic Force Fields for Nucleic Acids and Applications to Studies of Folding and Dynamics." *Curr. Opin. Struct. Biol.* 67: 9-17. (PMC7965779)

22. B.D. Ratnasinghe, A.M. Salsbury, and **J.A. Lemkul*** (2020) "Ion Binding Properties and Dynamics of the *bcl-2* G-Quadruplex Using a Polarizable Force Field." *J. Chem. Inf. Model.* 60 (12): 6476-6488. (PMC7775346)

23. A.M. Salsbury, T.J. Dean, and **J.A. Lemkul*** (2020) "Polarizable Molecular Dynamics Simulations of Two *c-kit* Promoter G-Quadruplexes: Effect of Primary and Secondary Structure on Loop and Ion Sampling." *J. Chem. Theory Comput.* 16 (5): 3430-3444. (PMC7221321)

24. **J.A. Lemkul*** (2020) "Same Fold, Different Properties: Polarizable Molecular Dynamics Simulations of Telomeric and TERRA G-Quadruplexes." *Nucleic Acids Res.* 48 (2): 561-575. (PMC6954416)

25. R. Pawlak, J.G. Vilhena, P. D'Astolfo, X. Liu, G. Prampolini, T. Meier, T. Glatzel, **J.A. Lemkul**, R. Häner, S. Decurtins, A. Baratoff, R. Pérez, S.-X. Liu, and E. Meyer (2020) "Sequential Bending and Twisting of C-C Bonds by Mechanical Lifting of a Pre-Adsorbed Polymer." *Nano Lett.* 20 (1): 652-657.

26. A.M. Salsbury, A.M. Brown, and **J.A. Lemkul*** (2019) "Integrating Scientific Programming in Communities of Practice for Students in the Life Sciences." *Proceedings of Practice & Experience in Advanced Research Computing (PEARC19)*, 6 pp. (Honorable Mention in "Workforce Development and Diversity" paper category)

27. A. Umana, **J.A. Lemkul**, and D.J. Slade (2019) "Complete genome of *Fusobacterium necrophorum* subsp. *necrophorum* ATCC 25286." *Microbiol. Resour. Announc*. 8 (8): e00025-19.

28. A.M. Salsbury and **J.A. Lemkul*** (2019) “Molecular Dynamics Simulations of the *c-kit1* Promoter G-Quadruplex: Importance of Electronic Polarization on Stability and Cooperative Ion Binding.” *J. Phys. Chem. B* 123 (1): 148-159.

29. **J.A. Lemkul*** (2019) “From Proteins to Perturbed Hamiltonians: A Suite of Tutorials for the GROMACS-2018 Molecular Simulation Package [Article v1.0].” *Living J. Comp. Mol. Sci.* 1 (1): 5068.

30. **J.A. Lemkul** and A.D. MacKerell, Jr. (2018) “Polarizable Force Field for RNA Based on the Classical Drude Oscillator.” *J. Comput. Chem.* 39 (32): 2624-2646. (PMC6284239)

31. D. van der Spoel, M.M. Ghahremanpour, and **J.A. Lemkul** (2018) “Small Molecule Thermochemistry: A Tool for Empirical Force Field Development.” *J. Phys. Chem. A* 122 (45): 8982-8988.

32. D.S. Davidson, A.M. Brown, and **J.A. Lemkul*** (2018) “Insights into Stabilizing Forces in Amyloid Fibrils of Differing Sizes from Polarizable Molecular Dynamics Simulations.” *J. Mol. Biol.* 430 (20): 3819-3834. (F1000 Prime Recommended paper)

33. B.E. Sanders, A. Umana, **J.A. Lemkul**, and D.J. Slade (2018) “FusoPortal: An interactive repository of hybrid MinION-sequenced *Fusobacterium* genomes improves gene identification and characterization.” *mSphere.* 3: e00228-18.

34. L.R. Hollingsworth IV, **J.A. Lemkul**, D.R. Bevan, and A.M. Brown (2018) “HIV-1 Env gp41 Transmembrane Domain Dynamics are Modulated by Lipid, Water, and Ion Interactions.” *Biophys. J.* 115 (1): 84-94.

Prior to starting at Virginia Tech

35. J. Huang, **J.A. Lemkul**, P.K. Eastman, and A.D. MacKerell, Jr. (2018) “Molecular Dynamics Simulations Using the Drude Polarizable Force Field on GPUs with OpenMM: Implementation, Validation, and Benchmarks.” *J. Comput. Chem.* 39 (21): 1682-1689. (PMC6031474)

36. E.H. Klontz, A.D. Tomich, S. Günther, **J.A. Lemkul**, D. Deredge, Z. Silverstein, J.F. Shaw, C. McElheny, Y. Doi, P. Wintrode, A.D. MacKerell, Jr., N. Sluis-Cremer, and E.J. Sundberg (2017) “Structure and dynamics of FosA-mediated fosfomycin resistance in *Klebsiella pneumonia* and *Escherichia coli*.” *Antimicrob. Agents and Chemother.* 61 (11): e01572-17. (PMC5655077)

37. **J.A. Lemkul** and A.D. MacKerell, Jr. (2017) “Polarizable Force Field for DNA Based on the Classical Drude Oscillator: I. Refinement Using Quantum Mechanical Base Stacking and Conformational Energetics.” *J. Chem. Theory Comput.* 13 (5): 2053-2071. (PMC5484419)

38. **J.A. Lemkul** and A.D. MacKerell, Jr. (2017) “Polarizable Force Field for DNA Based on the Classical Drude Oscillator: II. Microsecond Molecular Dynamics Simulations of Duplex DNA.” *J. Chem. Theory Comput.* 13 (5): 2072-2085. (PMC5485260)

39. **J.A. Lemkul** and A.D. MacKerell, Jr. (2016) “Balancing Interactions of Mg^{2+} in Aqueous Solution and with Nucleic Acid Moieties For a Polarizable Force Field Based on the Classical Drude Oscillator Model.” *J. Phys. Chem. B* 120 (44): 11436-11448. (PMC5148688)

40. **J.A. Lemkul**, S.K. Lakkaraju, and A.D. MacKerell, Jr. (2016) “Characterization of Mg^{2+} Distributions around RNA in Solution.” *ACS Omega* 1 (4): 680-688. (PMC5088455)

41. I. Soteras, F.-Y. Lin, K. Vanommeslaeghe, **J.A. Lemkul**, K.A. Armacost, C.L. Brooks III, and A.D. MacKerell, Jr. (2016) “Parametrization of Halogen Bonds in the CHARMM General Force Field: Improved Treatment of Ligand-Protein Interactions.” *Bioorg. Med. Chem.* 24 (20): 4812-4825. (PMC5053860)

42. **J.A. Lemkul**, J. Huang, B. Roux, and A.D. MacKerell, Jr. (2016) “An Empirical Polarizable Force Field Based on the Classical Drude Oscillator Model: Development History and Recent Applications.” *Chem. Rev.* 116 (9): 4983-5013. (PMC4865892)

43. J. Lee, X. Cheng, J. Swails, M.S. Yeom, P. Eastman, **J.A. Lemkul**, S. Wei, J. Buckner, J.C. Jeong, Y. Qi, S. Jo, V. Pande, D.A. Case, C.L. Brooks III, A.D. MacKerell, Jr., J.B. Klauda, and W. Im (2016) "CHARMM-GUI Input Generation for NAMD, GROMACS, AMBER, OpenMM, and CHARMM/OpenMM Simulations using the CHARMM Force Fields." *J. Chem. Theory Comput.* 12 (1): 405-413. (PMC4712441)

44. S.K. Lakkaraju, **J.A. Lemkul**, J. Huang, and A.D. MacKerell, Jr. (2016) "DIRECT-ID: An Automated Method to Identify and Quantify Conformational Variations - Application to β_2-adrenergic GPCR." *J. Comput. Chem.* 37 (4): 416-425. (PMC4756637)

45. **J.A. Lemkul**, J. Huang, and A.D. MacKerell, Jr. (2015) "Induced Dipole-Dipole Interactions Influence Unfolding Pathways of Wild-Type and Mutant Amyloid β-Peptides." *J. Phys. Chem. B* 119 (51): 15574-15582. (PMC4690896)

46. **J.A. Lemkul**, B. Roux, D. van der Spoel, and A.D. MacKerell, Jr. (2015) "Implementation of Extended Lagrangian Dynamics in GROMACS for Polarizable Simulations Using the Classical Drude Oscillator Model." *J. Comput. Chem.* 36 (19): 1473-1479. (PMC4481176)

47. **J.A. Lemkul**, S.N. Lewis, J. Bassaganya-Riera, and D.R. Bevan (2015) "Phosphorylation of PPARγ Affects Collective Motions of the PPARγ-RXRα-DNA Complex." *PLoS ONE.* 10 (5): e0123984.

48. S.R. Gerben, **J.A. Lemkul**, A.M. Brown, and D.R. Bevan (2014) "Comparing Atomistic Molecular Mechanics Force Fields for a Difficult Target: A Case Study of the Amyloid β-Peptide." *J. Biomol. Struct. Dyn.* 32 (11): 1817-1832.

49. **J.A. Lemkul**, A. Savelyev, and A.D. MacKerell, Jr. (2014) "Induced Polarization Influences the Fundamental Forces in DNA Base Flipping." *J. Phys. Chem. Lett.* 5 (12): 2077-2083. (PMC4064933)

50. D.G.S. Capelluto, X. Zhao, A. Lucas, **J.A. Lemkul**, S. Xiao, X. Fu, F. Sun, D.R. Bevan, and C.V. Finkielstein (2014) "Biophysical and molecular dynamics studies of phosphatidic acid binding to the Dvl-2 DEP domain." *Biophys. J.* 106 (5): 1101-1111.

51. A.M. Brown, **J.A. Lemkul**, N. Schaum, and D.R. Bevan (2014) "Simulations of Monomeric Amyloid β-Peptide (1-40) with Varying Solution Conditions and Oxidation State of Met35: Implications for Aggregation." *Arch. Biochem. Biophys.* 545 (1): 44-62.

52. **J.A. Lemkul** and D.R. Bevan (2013) "Aggregation of Alzheimer's Amyloid β-Peptide in Biological Membranes: A Molecular Dynamics Study." *Biochemistry.* 52 (29): 4971-4980.

53. **J.A. Lemkul*** and D.R. Bevan (2012) "The Role of Molecular Simulations in the Development of Inhibitors of Amyloid β-Peptide Aggregation for the Treatment of Alzheimer's Disease." *ACS Chem. Neurosci.* 3 (11): 845-856. (Cover art for special issue on Alzheimer's Disease)

54. **J.A. Lemkul** and D.R. Bevan (2012) "Morin Inhibits the Early Stages of Amyloid β-Peptide Aggregation by Altering Tertiary and Quaternary Interactions to Produce 'Off-Pathway' Structures." *Biochemistry.* 51 (30): 5990-6009.

55. **J.A. Lemkul** and D.R. Bevan (2011) "Lipid Composition Influences the Release of Alzheimer's Amyloid β-Peptide from Membranes." *Protein Sci.* 20 (9): 1530-1545.

56. **J.A. Lemkul** and D.R. Bevan (2011) "Characterization of Interactions Between PilA from *Pseudomonas aeruginosa* Strain K and a Model Membrane." *J. Phys. Chem. B* 115 (24): 8004-8008.

57. **J.A. Lemkul**, W.J. Allen, and D.R. Bevan (2010) "Practical Considerations for Building GROMOS-Compatible Small Molecule Topologies." *J. Chem. Inf. Model.* 50 (12): 2221-2235.

58. P. Mehere, Q. Han, **J.A. Lemkul**, C.J. Vavricka, H. Robinson, D.R. Bevan, and J. Li (2010) "Tyrosine Aminotransferase: biochemical and structural properties and molecular dynamics simulations." *Protein & Cell* 1 (11): 1023-1032.

59. **J.A. Lemkul** and D.R. Bevan (2010) "Destabilizing Alzheimer's $A\beta_{42}$ Protofibrils with Morin: Mechanistic Insights from Molecular Dynamics Simulations." *Biochemistry.* 49 (18): 3935-3946.

60. **J.A. Lemkul** and D.R. Bevan (2010) "Assessing the Stability of Alzheimer's Amyloid Protofibrils Using Molecular Dynamics." *J. Phys. Chem. B* 114 (4): 1652-1660. ("Editor Selected Biophysical Research," October 2011)

61. W.J. Allen, **J.A. Lemkul**, and D.R. Bevan (2009) "GridMAT-MD: A Grid-based Membrane Analysis Tool for Use With Molecular Dynamics." *J. Comput. Chem.* 30 (12): 1952-1958.

62. **J.A. Lemkul** and D.R. Bevan (2009) "Perturbation of membranes by the amyloid β-peptide – a molecular dynamics study." *FEBS J.* 276 (11): 3060-3075. (Highlighted in *FEBS J* virtual issue "Protein Misfolding, Prions, and Amyloid," January 2010)

63. **J.A. Lemkul** and D.R. Bevan (2008) "A Comparative Molecular Dynamics Analysis of the Amyloid β-Peptide in a Lipid Bilayer." *Arch. Biochem. Biophys.* 470 (1): 54-63.

BOOK CHAPTERS (*Corresponding author)

1. **J.A. Lemkul*** (2021) "Preparing and Analyzing Polarizable Molecular Dynamics Simulations with the Classical Drude Oscillator Model." In *Methods in Molecular Biology.* J. Mourão, I. Moreira, and M. Machuqueiro, Eds., 2315: 219-240.

2. **J.A. Lemkul*** (2020) "Pairwise-Additive and Polarizable Atomistic Force Fields for Molecular Dynamics Simulations of Proteins" *Computational Approaches for Understanding Dynamical Systems: Protein Folding and Assembly*. In *Progress in Molecular Biology and Translational Science*. B. Strodel and B. Barz, Eds., 170: 1-71.

PREPRINTS, IN PREPARATION, AND SUBMITTED MANUSCRIPTS (*Corresponding author)

1. H.M. Michel, M.D. Polêto, and **J.A. Lemkul*** "Running Gaussian-Accelerated Molecular Dynamics Simulations in NAMD [Article v1.0]" Submitted to *Living J. Comput. Mol. Sci.*

2. B. Grupp, J. Graser, J. Seifermann, S. Gerhardt, **J.A. Lemkul**, N. Johnsson, and T. Gronemeyer "Interface Integrity in Septin Protofilaments is Maintained by an Arginine Residue Conserved from Yeast to Man." Submitted to *Mol. Biol. Cell*. BioRxiv DOI: 10.1101/2025.01.29.635471

3. A.M. Brown* and **J.A. Lemkul*** "Robustness in Biomolecular Simulations: Addressing Challenges in Data Generation, Analysis, and Curation" Submitted to *Cell Rep Phys Sci.* ChemRxiv DOI: 10.26434/chemrxiv-2025-gx5p5

INVITED SEMINARS AND PRESENTATIONS

Since starting at Virginia Tech

1. "Polarizable Molecular Dynamics Simulations of Noncanonical Nucleic Acids" Genetics, Bioinformatics, and Computational Biology Seminar Series. October 2024.

2. "Electronic Polarization in Nucleic Acids: Implications for Structure, Dynamics, and Drug Design" MolSSI Minisymposium. July 2023.

3. "CHARMM Force Field Development History, Features, and Implementation in GROMACS" BioExcel Webinar Series. November 2021 (Virtual presentation via Zoom)

4. “Induced Electronic Polarization in RNA G-Quadruplexes and Tetraloop Folding” Telluride Science Research Center RNA Dynamics Workshop. July 2021. (Virtual presentation via Zoom)

5. “Conformational Dynamics and Ion-Binding Properties of DNA G-Quadruplexes from Polarizable Simulations with the Drude-2017 Force Field” Spring 2021 American Chemical Society National Meeting. April 2021. (Virtual presentation via Zoom)

6. “Dipole-Dipole Interactions Modulate Secondary and Tertiary Structure of Wild-Type and Mutant Amyloid β-Peptides” Spring 2021 American Chemical Society National Meeting. April 2021. (Virtual presentation via Zoom)

7. “Development of the Drude Nucleic Acid Force Field and Applications to G-Quadruplexes” University of Albany. Albany, NY, March 2021. (Virtual presentation via Zoom)

8. “Toward Computational Drug Design Against DNA G-Quadruplexes: Insights from Molecular Dynamics Simulations” Virginia Tech Life Sciences Seminar Series. Blacksburg, VA, October 2020.

9. “Development of the Drude Polarizable Force Field for DNA and RNA and Applications to Investigations of Nucleic Acid Structure and Dynamics” Spring 2020 American Chemical Society National Meeting. Philadelphia, PA, March 2020. (Conference canceled due to COVID-19, delivered online)

10. “Influence of Induced Polarization on the Dynamics and Folding Free Energy of the Amyloid β-Peptide.” Spring 2020 American Chemical Society National Meeting. Philadelphia, PA, March 2020. (Contributed oral presentation, Conference canceled due to COVID-19, delivered online)

11. “Properties of DNA and RNA G-Quadruplexes from Polarizable Simulations” Virginia Tech Center for Drug Discovery Annual Workshop. Blacksburg, VA, January 2020.

12. “Development of the Drude-2017 Force Field for DNA and RNA” CECAM workshop – Beyond point charges: novel electrostatic developments in force fields. Swiss Federal Institute of Technology. Lausanne, Switzerland, December 2019.

13. “Drude Polarizable Force Field for Nucleic Acids: Development and Application to G-Quadruplexes” University of Rochester Bioinformatics Cluster Monthly Seminar. Rochester, NY, May 2019.

14. “Insights into DNA and RNA G-Quadruplexes from Polarizable Molecular Dynamics Simulations.” Spring 2019 American Chemical Society National Meeting. Orlando, FL, April 2019.

Prior to starting at Virginia Tech

15. “Polarizable Force Field for DNA and RNA Based on the Classical Drude Oscillator Model.” Telluride Science Research Center. Telluride, CO, June 2017.

16. “Polarizable Force Field for DNA and RNA Based on the Classical Drude Oscillator Model.” National Institutes of Health, Laboratory of Computational Biology. Rockville, MD, April 2016.

17. “Influence of Induced Polarization on Amyloid Peptide Misfolding in Different Solution Environments.” Spring 2015 American Chemical Society National Meeting. Denver, CO, March 2015.

18. “Biomolecular Force Fields: Fundamentals and Improvements for the Next Generation.” 8th Annual q-bio Summer School, University of New Mexico, Albuquerque, NM, August 2014.

19. “Insights into Protein Complexation and Drug Discovery from Steered Molecular Dynamics Simulations.” 2013 GROMACS Workshop and Conference, Charlottesville, VA, September 2013.

20. “Molecular Dynamics Simulations: Using High-Performance Computing to Solve Problems in Biology, Chemistry, and Physics.” Roanoke College, Salem, VA, March 2013.

21. "Dimerization of the Amyloid β-Peptide in Biological Membranes." CECAM workshop – Anchoring simulations to experiments: challenges for understanding and treating Alzheimer's disease. Insitut de Biologie Physico-Chemique. Paris, France, May 2012.

22. "Advancing Therapeutics for Alzheimer's Disease with Molecular Dynamics Simulations: An Unconventional Approach to Drug Discovery." Washington & Lee University, Lexington, VA, December 2010.

23. "Computational Approaches to Alzheimer's Drug Discovery." University of Virginia, Charlottesville, VA, November 2010.

24. "Advancing Therapeutics for Alzheimer's Disease with Molecular Dynamics Simulations." 2010 meeting of the Virginia Academy of Science (88th VAS), James Madison University, Harrisonburg, VA, May 2010.

POSTERS AND CONFERENCE PRESENTATIONS

Since starting at Virginia Tech

1. **J.A. Lemkul** "Development of a polarizable force field for phosphorylated proteins and polypeptides" Spring 2025 American Chemical Society National Meeting, San Diego, CA, March 2025. (Oral presentation)

2. **J.A. Lemkul** "Development of a polarizable force field for phosphorylated proteins and polypeptides" Biophysical Society 69th Annual Meeting, Los Angeles, CA, February 2025.

3. **J.A. Lemkul** "Electric Fields and Induced Polarization Effects in RNA: Implications for Folding and Function" Spring 2024 American Chemical Society National Meeting, New Orleans, LA, March 2024.

4. **J.A. Lemkul** "Electric Fields and Induced Polarization Effects in RNA: Implications for Folding and Function" Biophysical Society 68th Annual Meeting, Philadelphia, PA, February 2024.

5. **J.A. Lemkul** "Electric Fields in Noncanonical Nucleic Acids from Drude Polarizable Simulations" CHARMM Developers' Annual Meeting. University of Michigan. Ann Arbor, MI, July 2023. (Oral presentation)

6. **J.A. Lemkul** "Electric Fields and Induced Polarization Effects in RNA" CECAM workshop – RNA dynamics from experimental and computational approaches. Swiss Federal Institute of Technology. Insitut de Biologie Physico-Chemique. Paris, France, June 2023. (Oral presentation)

7. **J.A. Lemkul**, M.D. Polêto, and H.M. Michel "Electric Field Effects in DNA G-Quadruplexes Drive Ion Binding" Fall 2022 American Chemical Society National Meeting. Chicago, IL, August 2022. (Poster)

8. **J.A. Lemkul** "Nucleic Acid and Amyloidogenic Protein Folding and Dynamics using a Polarizable Force Field Based on the Classical Drude Oscillator Model." Spring 2020 American Chemical Society National Meeting. Philadelphia, PA, March 2020. (Poster, Conference canceled due to COVID-19, delivered online)

9. **J.A. Lemkul** "Polarizable Molecular Dynamics Simulations of DNA G-Quadruplexes Reveal Different Properties of Nucleobase Electronic Structure and Cation Binding." Biophysical Society 64th Annual Meeting, San Diego, CA, February 2020. (Poster)

10. **J.A. Lemkul**, A.M. Salsbury, D.S. Davidson, Y. Yu, and A.M. Brown "Influence of Electronic Polarization on the Structure and Energetics of Proteins and Nucleic Acids" Computational Chemistry Gordon Research Conference, July 2018. (Poster and selected for "flash talk")

11. **J.A. Lemkul** and A.D. MacKerell, Jr. "Polarizable Force Field for RNA Based on the Classical Drude Oscillator Model." Fall 2017 American Chemical Society National Meeting, Washington, DC, August 2017. (Poster)

Prior to starting at Virginia Tech

12. **J.A. Lemkul** and A.D. MacKerell, Jr. "Polarizable Force Field for DNA and RNA Based on the Classical Drude Oscillator Model." Fall 2016 American Chemical Society National Meeting, Philadelphia, PA, August 2016. (Poster)

13. **J.A. Lemkul** and A.D. MacKerell, Jr. "Polarizable Force Field for DNA and RNA Based on the Classical Drude Oscillator Model." School of Pharmacy Research Day, Baltimore, MD, April 2016. (1st Place poster, Pharmaceutical Sciences Postdoc category)

14. **J.A. Lemkul**, A. Savelyev, and A.D. MacKerell, Jr. "Towards a Polarizable Force Field for RNA Based on the Classical Drude Oscillator." School of Pharmacy Research Day, Baltimore, MD, April 2015. (Poster)

15. **J.A. Lemkul**, A. Savelyev, and A.D. MacKerell, Jr. "Towards a Polarizable Force Field for RNA Based on the Classical Drude Oscillator," *Biophys. J.* 108 (S1): 159a. February 2015. (Poster presentation, given at the Biophysical Society 59th Annual Meeting, Baltimore, MD)

16. **J.A. Lemkul**, A. Savelyev, and A.D. MacKerell, Jr. "Induced Polarization Influences the Fundamental Forces in DNA Base Flipping" School of Pharmacy Research Day, Baltimore, MD, April 2014. (Poster)

17. **J.A. Lemkul** and D.R. Bevan "New Insights into the Mechanism of Alzheimer's Disease from Molecular Dynamics Simulations." Spring ICTAS Doctoral Scholars Meeting, Blacksburg, VA, April 2012. (Poster)

18. **J.A. Lemkul** and D.R. Bevan "Lipid Composition Influences the Release of Alzheimer's Amyloid β-Peptide from Membranes." Spring ICTAS Doctoral Scholars Meeting, Blacksburg, VA, April 2011. (Poster)

19. **J.A. Lemkul** and D.R. Bevan "Ganglioside GM1 Facilitates Release of Alzheimer's Aβ Peptide from Lipid Rafts." ACC Interdisciplinary Forum for Discovery in Life Sciences, Blacksburg, VA, October 2010. (Oral presentation)

20. **J.A. Lemkul** and D.R. Bevan "Ganglioside GM1 Facilitates Release of Alzheimer's Aβ Peptide from Lipid Rafts." 2010 ICTAS Research Day, Blacksburg, VA, September 2010. (Poster)

21. **J.A. Lemkul** and D.R. Bevan "Thermodynamics of Amyloid Fibril Dissociation: Identifying Targets for Therapeutic Intervention in Alzheimer's Disease." Edward Via College of Osteopathic Medicine 6th Annual Research Day, Blacksburg, VA, October 2009. (1st Place Student Biomedical poster, oral presentation)

22. **J.A. Lemkul** and D.R. Bevan "Dissolving Alzheimer's Amyloid Plaques with Red Wine: Insights from Molecular Dynamics Simulations." *Protein Sci.* 18 (S1): 73. 23rd Annual Symposium of the Protein Society, Boston, MA, July 2009. (Poster)

23. **J.A. Lemkul** and D.R. Bevan "Dissolving Alzheimer's Amyloid Plaques with Red Wine: Insights from Molecular Dynamics Simulations." 4th Annual Virginia Tech Structural Biology Symposium, Blacksburg, VA, March 2009. (Poster)

24. **J.A. Lemkul** and D.R. Bevan "Dissolving Alzheimer's Amyloid Plaques with Red Wine: Insights from Molecular Dynamics Simulations." 25th Annual Graduate Student Association Research Symposium, Blacksburg, VA, March 2009. (Poster)

25. **J.A. Lemkul** and D.R. Bevan "Binding of Flavonoids to the Amyloid β-Peptide: Treating Alzheimer's Disease with Red Wine." *Free Radic. Biol. Med.* 45 (1): S87. Suppl. 16th Annual Meeting of the Society for Free Radical Biology and Medicine, November 2008. (Poster)

26. **J.A. Lemkul** and D.R. Bevan "Membrane Molecular Dynamics of Alzheimer's Amyloid-β Peptide." Dean's Forum on Health, Food, and Nutrition, Blacksburg, VA, November 2007. (Poster)

27. **J.A. Lemkul** and D.R. Bevan "Membrane Molecular Dynamics of Alzheimer's Amyloid-β Peptide." 2007 MII Technical Conference and Review, Blacksburg, VA, October 2007. (Poster)

28. **J.A. Lemkul** and D.R. Bevan "A Molecular Dynamics Analysis of the Amyloid-β Peptide: Insights into the Molecular Mechanism of Alzheimer's Disease." *Protein Sci.* 16 (S1): 79. 21st Annual Symposium of the Protein Society, Boston, MA, July 2007. (Poster and oral presentation)

29. **J.A. Lemkul**, A.E. Tanner, and K.E. Saker "The Effect of Antioxidants on 8-Oxoguanine Levels in the Treatment of Feline Obesity and Human Cancer," Summer Undergraduate Research Program Symposium, Blacksburg, VA, August 2006. (Oral presentation)

LAB MEMBER AND COLLABORATOR POSTERS, PRESENTATIONS, AND PUBLISHED PROCEEDINGS

(Presenters underlined, *Undergraduate student, **Graduate student)

1. L.I. Gil Pineda** and **J.A. Lemkul** (2025) "Enhanced Sampling of Phosphorylated Intrinsically Disordered Proteins: A Computational Study on β-Catenin" *Spring 2025 American Chemical Society National Meeting*. San Diego, CA.

2. E. Mohammadi,** H.M. Michel,** and **J.A. Lemkul** (2025) "Computational Approaches in Drug Discovery for Type 2 Diabetes Mellitus: Targeting Key Enzymes in Carbohydrate Digestion" *Spring 2025 American Chemical Society National Meeting*. San Diego, CA.

3. H.M. Michel,** A.D. MacKerell Jr., and **J.A. Lemkul** (2025) "Advancing Drug Targeting of DNA and RNA Structures using Polarizable Mixed-Solvent Simulations" *Spring 2025 American Chemical Society National Meeting*, San Diego, CA.

4. L.I. Gil Pineda** and **J.A. Lemkul** (2025) "Enhanced Sampling of Phosphorylated Intrinsically Disordered Proteins: A Computational Study on β-Catenin" *69th Annual Meeting of the Biophysical Society.* Los Angeles, CA.

5. A.M. Goodberlet** and **J.A. Lemkul** (2025) "Characterizing the Conformational Landscape of $A\beta_{10-35}$ from Weighted Ensemble Simulations with the Drude Polarizable Force Field" *69th Annual Meeting of the Biophysical Society.* Los Angeles, CA.

6. K.B. Malewicz,** J.M. Montgomery,** J.W. McGlothlin, and **J.A. Lemkul** (2025) "Decoding Dynamics to Understand Nature: What Sets Garter Snake Sodium Channels Apart in Their Fight Against Tetrodotoxin?" *69th Annual Meeting of the Biophysical Society.* Los Angeles, CA.

7. P.C. Gilles,* L.I. Gil Pineda,** and **J.A. Lemkul** (2025) "Deciphering Phosphorylation-Induced Changes in α-Synuclein Structure using Drude Polarizable Simulations" *69th Annual Meeting of the Biophysical Society*. Los Angeles, CA.

8. H.M. Michel,** A.D. MacKerell Jr., and **J.A. Lemkul** (2025) "Advancing Drug Targeting of DNA and RNA Structures using Polarizable Mixed-Solvent Simulations" *69th Annual Meeting of the Biophysical Society.* Los Angeles, CA.

9. H.M. Michel,** A.D. MacKerell, Jr., and **J.A. Lemkul** (2024) "Advancing Targeting of DNA and RNA Structures Using Polarizable Simulations and SILCS" *Computational Medicinal Chemistry School.* Cambridge, MA.

10. H.M. Michel,** S.M. Morlatt,* and **J.A. Lemkul** (2024) "Harnessing Polarizable Simulations and SILCS for Computer-Aided Drug Design Against the LTR-III G-Quadruplex" *Computational Chemistry Gordon Research Seminar and Gordon Research Conference.* Portland, ME.

11. K.B. Malewicz,** J.M. Montgomery,** J.W. McGlothlin, and **J.A. Lemkul** (2024) "Understanding Extreme Toxin Resistance in Garter Snakes using Molecular Dynamics Simulations" *3rd Joint Conference on Evolutionary Biology.* Montreal, QC, Canada.

12. C.J. Miller,* L.I. Gil Pineda,** and **J.A. Lemkul** (2024) "Characterizing the Electronic Impact of Phosphorylation on GSXS Tetrapeptides" *Dennis Dean Undergraduate Research and Creative Scholarship Conference.* Blacksburg, VA.

13. S.M. Morlatt,* H.M. Michel,** and **J.A. Lemkul** (2024) "Computer-Aided Drug Design for HIV-1 by Exploiting Differences in *LTR-III* G-Quadruplex Conformations" *Dennis Dean Undergraduate Research and Creative Scholarship Conference.* Blacksburg, VA.

14. R. DeHority, L.I. Gil Pineda,** K. Cochran, **J.A. Lemkul**, and C. Zhang (2024) "pH-Dependent Specificity in Cysteine Proteases" *Fall 2024 American Chemical Society National Meeting,* Denver, CO. (Platform presentation)

15. M.D. Polêto and **J.A. Lemkul** (2024) "Optimizing PET biorecycling solutions through electronically polarizable simulations" *Spring 2024 American Chemical Society National Meeting*, New Orleans, LA.

16. H.M. Michel,** S. Morlatt,* and **J.A. Lemkul** (2024) "Advancing G-Quadruplex Drug Targeting Through Polarizable Simulations and SILCS" *Spring 2024 American Chemical Society National Meeting*, New Orleans, LA.

17. L.I. Gil Pineda,** K.M. King, **J.A. Lemkul**, and A.M. Brown (2024) "Characterizing $A\beta_{16-22}$ Aggregation Pathways Through Molecular Dynamics Simulations" *68th Annual Meeting of the Biophysical Society*. Philadelphia, PA.

18. S. Farrokhpoor,** H.M. Michel,** M.D. Polêto, and **J.A. Lemkul** (2024) "Comparing Enhanced Sampling Strategies to Study Reversible Folding of the UUCG RNA Tetraloop with the Drude Polarizable Force Field" *68th Annual Meeting of the Biophysical Society*. Philadelphia, PA.

19. C.J. Miller,* L.I. Gil Pineda,** and **J.A. Lemkul** (2024) "Characterizing the Electronic Impact of Phosphorylation on GSXS Tetrapeptides" *68th Annual Meeting of the Biophysical Society*. Philadelphia, PA.

20. E. Mohammadi** and **J.A. Lemkul** (2024) "Insights into the Electronic and Structural Properties of Cellulose and Amylose: A Comparative Force Field Study" *68th Annual Meeting of the Biophysical Society*. Philadelphia, PA.

21. R. Fogarty,** H.M. Michel,** and **J.A. Lemkul** (2024) "Investigating Potential Drug Targets in the *PIM1* Promoter G-Quadruplex" *68th Annual Meeting of the Biophysical Society*. Philadelphia, PA.

22. A.M. Goodberlet** and **J.A. Lemkul** (2024) "The Conformational Landscape of $A\beta_{10-35}$ from Conventional and Weighted Ensemble Simulations with the Drude Polarizable Force Field" *68th Annual Meeting of the Biophysical Society*. Philadelphia, PA.

23. K. Malewicz,** J.M. Montgomery,** J.W. McGlothlin, and **J.A. Lemkul** (2024) "From Evolution to Dynamics: Understanding Tetrodotoxin Resistance in Garter Snakes at the Molecular Level" *68th Annual Meeting of the Biophysical Society*. Philadelphia, PA.

24. H.M. Michel,** S. Morlatt,* and **J.A. Lemkul** (2024) "Advancing G-Quadruplex Drug Targeting Through Polarizable Simulations and SILCS" *68th Annual Meeting of the Biophysical Society*. Philadelphia, PA.

25. M.D. Polêto and **J.A. Lemkul** (2024) "Optimizing PET biorecycling solutions through electronically polarizable simulations" *68th Annual Meeting of the Biophysical Society*. Philadelphia, PA.

26. J.M. Montgomery** and **J.A. Lemkul** (2024) "Investigating the Electrostatic Forces Influencing the Structure and Dynamics of the Beta-2 Adrenergic Receptor and WALP Peptide" *68th Annual Meeting of the Biophysical Society*. Philadelphia, PA.

27. J.M. Montgomery** and **J.A. Lemkul** (2023) "Partitioning Free Energies and Induced Dipole Response of Small Molecules Across a POPC Membrane using Polarizable Molecular Dynamics" *Fall 2023 American Chemical Society National Meeting.* San Francisco, CA.

28. K. Malewicz,** J.M. Montgomery,** J.W. McGlothlin, and **J.A. Lemkul** (2023) "Using Molecular Dynamics to Connect Genotype to Phenotype" *SMBE23.* Ferrera, Italy.

29. R. DeHority, L.I. Gil Pineda,** K. Cochran, Y. Bian, **J.A. Lemkul**, and C. Zhang (2023) "In vitro validation of Cathepsin S docking models" *Immunology 2023.* Washington, DC.

30. M.D. Polêto and **J.A. Lemkul** (2023) "Modulation of Polyethylene Terephthalate (PET) Electronic Properties by PET-Degrading Enzymes" *Spring 2023 American Chemical Society National Meeting.* Indianapolis, IN. (Platform talk)

31. M.D. Polêto and **J.A. Lemkul** (2023) "Active-Site Electronic Properties and Conformational Dynamics of PET-Degrading Enzymes" *67th Annual Meeting of the Biophysical Society.* San Diego, CA.

32. L.I. Gil Pineda** and **J.A. Lemkul** (2023) "Using Tetrapeptide GSSS and β-catenin$^{17-48}$ to Study the Effects of Phosphoserine on Polypeptide Conformational Ensembles" *67th Annual Meeting of the Biophysical Society.* San Diego, CA.

33. J.M. Montgomery** and **J.A. Lemkul** (2023) "Partitioning Free Energies and Induced Dipole Response of Small Molecules Across a POPC Membrane using Polarizable Molecular Dynamics" *67th Annual Meeting of the Biophysical Society.* San Diego, CA.

34. H.M. Michel** and **J.A. Lemkul** (2023) "Determining the Conformational Ensemble of the HIV-1 LTR G-Quadruplexes using Gaussian-Accelerated Molecular Dynamics" *67th Annual Meeting of the Biophysical Society.* San Diego, CA.

35. R. Fogarty,** H.M. Michel,** and **J.A. Lemkul** (2023) "Dynamics and Conformational Heterogeneity of the PIM1 G-Quadruplex from Polarizable Molecular Dynamics Simulations" *67th Annual Meeting of the Biophysical Society.* San Diego, CA.

36. H.M. Michel** and **J.A. Lemkul** (2022) "A Tale of Two Loops: Characterization of Two G-Quadruplexes in the HIV-1 Long Terminal Repeat Using Polarizable Molecular Dynamics Simulations" *G4thering*, Marienbad, Czech Republic.

37. K.S. Amin, **J.A. Lemkul**, A.D. MacKerell, D. Salahub, and S. Noskov (2022) "Improved Monovalent Cation-Protein Interactions in the CHARMM Drude Polarizable Force Field" *Biophysics at the Dawn of Exascale Computers*, Hamburg, Germany.

38. S. Noskov, S.K. Amin, A.D. MacKerell, D.R. Salahub, and **J.A. Lemkul** (2022) "Drude Polarizable Model of Monovalent Cation-Protein Interactions" *12th Triennial Congress of the World Association of Theoretical Chemistry 2022*, Vancouver, Canada. (Contributed oral presentation)

39. R. Fogarty,* H.M. Michel,** S. Farrokhpoor,* and **J.A. Lemkul** (2022) "Molecular Dynamics Simulations of the Human VEGF Promoter G-Quadruplex" *Dennis Dean Undergraduate Research and Creative Scholarship Conference.* Blacksburg, VA.

40. M.D. Polêto and **J.A. Lemkul** (2022) "Ion Binding Free-Energy Landscapes for Telomeric and TERRA G-Quadruplexes" *66th Annual Meeting of the Biophysical Society.* San Francisco, CA.

41. H.M. Michel** and **J.A. Lemkul** (2022) "A Tale of Two Loops: Polarizable Molecular Dynamics Simulations of Two HIV-1 LTR G-Quadruplexes" *66th Annual Meeting of the Biophysical Society.* San Francisco, CA.

42. L.I. Gil Pineda** and **J.A. Lemkul** (2022) "Going Through Changes: Effect of Phosphoserine on Secondary Structure Preference and Dipole-Dipole Interactions in Model Peptides" *66th Annual Meeting of the Biophysical Society.* San Francisco, CA.

43. D.S. Davidson** and **J.A. Lemkul** (2022) "Reputation for Aggregation: Effect of Pyroglutamylation on the Amyloid β-Peptide" *66th Annual Meeting of the Biophysical Society.* San Francisco, CA. (Platform talk)

44. J.M. Montgomery** and **J.A. Lemkul** (2022) "Polarization in Partitioning: Quantifying the Effects of Induced Dipoles on Amino Acid Sidechain Analogs in a POPC Membrane" *66th Annual Meeting of the Biophysical Society.* San Francisco, CA. (Platform talk)

45. R. Fogarty,* H.M. Michel,** S. Farrokhpoor,* and **J.A. Lemkul** (2022) "Molecular Dynamics Simulations of the Human VEGF Promoter G-Quadruplex" *66th Annual Meeting of the Biophysical Society.* San Francisco, CA.

46. S.K. Amin, A.D. MacKerell, **J.A. Lemkul**, D.R. Salahub, and S. Noskov (2021) "Multi-scale parametrization of non-bonded interactions in the Drude polarizable force-field." *IUPAC CCCE 2021*. Virtual.

47. B.D. Ratnasinghe,** A.M. Salsbury,** and **J.A. Lemkul** (2021) "Ion Binding to the *bcl-2* G-Quadruplex from Polarizable Simulations with the Drude Force Field" *65th Annual Meeting of the Biophysical Society.* Virtual.

48. A.N. Corrigan** and **J.A. Lemkul** (2021) "Drude Polarizable Simulations of the p53 Transactivation Domain with Different Binding Partners" *65th Annual Meeting of the Biophysical Society.* Virtual.

49. D.S. Davidson,** J.A. Kraus,* J.M. Montgomery,** and **J.A. Lemkul** (2020) "Effect of Familial Alzheimer's Disease Mutations on the Folding Free Energy of the Amyloid β-Peptide" *259th American Chemical Society National Meeting.* Philadelphia, PA. (Conference canceled due to COVID-19, delivered online)

50. A.M. Salsbury** and **J.A. Lemkul** (2020) "Influence of Monovalent Cations on the Dynamics of the *c-kit1* Promoter G-Quadruplex using Polarizable Molecular Dynamics Simulations" *259th American Chemical Society National Meeting.* Philadelphia, PA. (Conference canceled due to COVID-19, delivered online)

51. T. Dean,* A.M. Salsbury,** and **J.A. Lemkul** (2020) "Dynamics of the 1:2:1 and 1:6:1 *c-myc* G-Quadruplexes using the Drude Polarizable Force Field" *64th Annual Meeting of the Biophysical Society.* San Diego, CA.

52. D.S. Davidson,** J.A. Kraus,* J.M. Montgomery,** and **J.A. Lemkul** (2020) "Effect of Familial Alzheimer's Disease Mutations on the Folding Free Energy of the Amyloid β-Peptide" *64th Annual Meeting of the Biophysical Society.* San Diego, CA. (Selected for "flash talk")

53. A.M. Salsbury** and **J.A. Lemkul** (2020) "Influence of Monovalent Cations on the Dynamics of the *c-kit1* Promoter G-Quadruplex using Polarizable Molecular Dynamics Simulations" *64th Annual Meeting of the Biophysical Society.* San Diego, CA.

54. B.D. Ratnasinghe,* A.M. Salsbury,** and **J.A. Lemkul** (2020) "Polarizable Molecular Dynamics Simulations of an RNA Duplex:G-Quadruplex Junction in Complex with the Fragile X Mental Retardation Protein" *64th Annual Meeting of the Biophysical Society.* San Diego, CA.

55. J.A. Kraus,* K.M. Wysong,* D.S. Davidson**, and **J.A. Lemkul** (2019) "The Effects of Charge-Altering Modifications on Amyloidogenic Proteins using Molecular Dynamics Simulations" *7th Annual Virginia Tech Center for Drug Discovery Poster Session*. Blacksburg, VA.

56. J.A. Kraus,* K.M. Wysong,* D.S. Davidson**, and **J.A. Lemkul** (2019) "The Effects of Charge-Altering Modifications on Amyloidogenic Proteins using Molecular Dynamics Simulations" *Engelpalooza Undergraduate Research Showcase*. Blacksburg, VA.

57. A.M. Salsbury,** **J.A. Lemkul**, and A.M. Brown (2019) "Application of GPU-Accelerated Molecular Dynamics Simulations of G-Quadruplexes with the Drude Polarizable Force Field" *Practice and Experience in Advanced Research Computing (PEARC19)*. Chicago, IL.

58. B.D. Ratnasinghe,* A.M. Salsbury,** D.L. Porier,* and **J.A. Lemkul** (2019) "Structure and Dynamics of the *bcl-2* Promoter G-Quadruplex using the Drude Polarizable Force Field" *700th Section Meeting of the Blue Ridge Section of the American Chemical Society*. Radford, VA.

59. T. Dean,* A.M. Salsbury,** and **J.A. Lemkul** (2019) "Structure and Dynamics of the *c-myc* G-Quadruplex" *Dennis Dean Undergraduate Research and Creative Scholarship Conference.* Blacksburg, VA.

60. D.S. Davidson** and **J.A. Lemkul** (2019) "Investigating the Role of Charge-Altering Post-Translational Modifications on Tau Peptide Conformational Ensembles using Polarizable Molecular Dynamics Simulations" *63rd Annual Meeting of the Biophysical Society.* Baltimore, MD.

61. B.D. Ratnasinghe,* A.M. Salsbury,** D.L. Porier,* and **J.A. Lemkul** (2019) "Structure and Dynamics of the *bcl-2* Promoter G-Quadruplex using the Drude Polarizable Force Field" *63rd Annual Meeting of the Biophysical Society.* Baltimore, MD.

62. L.R. Hollingsworth IV,* **J.A. Lemkul**, D.R. Bevan, R.D. Gandour, and A.M. Brown (2019) "Molecular Dynamics Simulations of gp120 and gp41 of HIV Env Provide Insights into Strain Specificity and the Role of the Membrane Environment" *63rd Annual Meeting of the Biophysical Society.* Baltimore, MD.

63. A.M. Salsbury** and **J.A. Lemkul** (2019) "Polarizable Molecular Dynamics Simulations of *c-kit* Oncogene Promoter G-Quadruplexes of Distinct Conformations" *63rd Annual Meeting of the Biophysical Society.* Baltimore, MD.

64. A. Salsbury,** B. Ratnasinghe,* J. Pinkman,* D. Porier,* and **J. Lemkul** (2018) "Influence of Electronic Polarization on the Structure and Dynamics of G-Quadruplexes with Distinct Folded Topologies" *6th Annual Virginia Tech Center for Drug Discovery Poster Session*. Blacksburg, VA.

65. B.D. Ratnasinghe,* A.M. Salsbury,** D.L. Porier,* and **J.A. Lemkul** (2018) "Influence of Electronic Polarization on RNA and DNA G-Quadruplex Structure and Dynamics" *Virginia Tech Annual Summer Research Symposium.* Blacksburg, VA.

66. D.S. Davidson,** A.M. Brown, and **J.A. Lemkul** (2018) "Insights into Stabilizing Forces in Amyloid Fibrils of Differing Sizes from Polarizable Molecular Dynamics Simulations" *University of Maryland Computer-Aided Drug Design Center Biennial Symposium.* Baltimore, MD.

67. A.M. Salsbury,** B. Ratnasinghe,* J. Pinkman,* D. Porier,* and **J.A. Lemkul** (2018) "Influence of Electronic Polarization on G-Quadruplex Structure and Dynamics" *University of Maryland Computer-Aided Drug Design Center Biennial Symposium.* Baltimore, MD.

68. Y. Yu, H. Chon,* H. Nguyen,* and **J.A. Lemkul** (2018) "Helix-Coil Equilibrium in Alanine-based Model Peptides: Implications for Protein Folding" *University of Maryland Computer-Aided Drug Design Center Biennial Symposium.* Baltimore, MD.

COURSES TAUGHT

Fall 2024 – Present	BCHM 5224 Protein Structure and Function (3 credits, 50% responsibility)
Spring 2021 – Present	BCHM 4554 Biophysics for Biochemistry (3 credits)
Spring 2018 – Spring 2019	BCHM 4784/5784 Advanced Applications in Molecular Life Sciences (3 credits)

CURRENT GRANT FUNDING

National Institutes of Health (NIGMS) 8/1/2019-6/30/2029 2.00 summer
R35GM133754 $2,954,101
Exploring the Role of Electronic Polarization in Biomolecular Folding and Interactions
Role: PI

U.S. Department of Energy 9/1/2021-8/31/2027 0.25 summer
DE-SC0022338 $1,010,000 (Lemkul share: $92,574)
Understanding the Biosynthesis and Functions of Modified F_{430} Coenzymes in Methanogens and Anaerobic Methanotrophs
Role: Co-PI (K.D. Allen, PI)

National Science Foundation 8/1/2020-7/31/2025 0.25 summer
DMR1933525 $25M (Lemkul share: $83,966)
MIP: GlycoMIP – Automating the Synthesis of Rationally Designed Glycopeptides
Role: Other Senior Personnel (M. Roman, PI)

COMPLETED GRANT FUNDING

Thomas F. and Kate Miller Jeffress Memorial Trust 6/30/2019-8/30/2021 1.41 summer
$120,000
Towards Computational Drug Design Against DNA G-Quadruplexes
Role: PI

National Institutes of Health (NIGMS) 3/1/2014-2/28/2017 12.00 calendar
F32GM109632 $163,726
Exploring RNA Folding and Dynamics Using a Polarizable Force Field
Role: PI

JOURNAL REVIEWER

ACS Chemical Neuroscience
ACS Omega
Advances in Bioinformatics
BBA Biomembranes
BBA General Subjects
BBA Proteins and Proteomics
Bioinformatics
Biophysical Journal
Computational and Structural Biotechnology Journal
Computational Biology and Chemistry
Expert Opinion on Drug Discovery
Interdisciplinary Sciences: Computational Life Sciences
International Journal of Biological Macromolecules
Journal of the American Chemical Society
Journal of Biomolecular Structure and Dynamics
Journal of Chemical Information and Modeling
Journal of Chemical Physics
Journal of Chemical Theory and Computation
Journal of Computational Chemistry
Journal of Molecular Modeling
Journal of Physical Chemistry
Journal of Physical Chemistry Letters
Molecular Informatics
Molecular Simulation
Molecules
Nature Communications
Nucleic Acids Research
PLoS Computational Biology
PloS ONE
Proteins: Structure, Function and Bioinformatics
Research on Chemical Intermediates
RSC Advances
Scientific Reports
SoftwareX
The Science of Nature (formerly Naturwissenschaften)

GRANT REVIEWER

2024	National Science Foundation Small Business Innovation Research (ad hoc)
2022	National Science Foundation Chemistry of Life Processes CAREER (ad hoc)
2022	National Science Foundation Matter and Materials Theory (ad hoc)
2022	American Chemical Society Petroleum Research Fund (ad hoc)
2020	Partnership for Advanced Computing in Europe (ad hoc)
2019	National Fund for Scientific and Technological Development (FONDECYT, Chile) (ad hoc)
2017	Defense Threat Reduction Agency (ad hoc)

EDITORIAL AND OTHER PROFESSIONAL SERVICE

2024	Co-Organizer, *Journal of Computational Chemistry* Special Issue in Honor of Alexander MacKerell Jr.'s 65th Birthday
2024	Platform session co-chair (Molecular Dynamics I), Biophysical Society National Meeting
2024	Executive Guest Editor, *Archives of Biochemistry and Biophysics* Special Issue: Dynamics of Small Molecule-Enzyme Interactions
2021	Co-organizer, "Recent Advances in Molecular Force Fields" COMP symposium, ACS Spring National Meeting

POSTDOCTORAL ASSOCIATES

Marcelo D. Polêto	December 2020 – August 2024	Currently: Postdoc, São Paulo University
Yue (Amira) Yu	January 2018 – November 2018	Currently: Senior Research Facilitator, UC Merced

PH.D. STUDENTS

Darcy S. Davidson	Biochemistry	Fall 2017 – Spring 2022
Dissertation:	*"Investigating the Electrostatic Properties and Dynamics of Amyloidogenic Proteins with Polarizable Molecular Dynamics Simulations"*	
Laura I. Gil Pineda	Biochemistry	Spring 2021 – Present
Ashley M. Goodberlet	Biochemistry	Fall 2022 – Present
Rakshitha R. Hosahalli	Biochemistry	Fall 2023 – Present
Haley M. Michel	Biochemistry	Fall 2020 – Present
Dissertation:	*"Computer-Aided Drug Design of G-Quadruplex Structures: Harnessing Electronic Polarization for Rational Drug Design"*	
Esmat Mohammadi	Chemical Engineering	Fall 2023 – Present
Julia M. Montgomery	Biochemistry	Fall 2019 – Summer 2024
Dissertation:	*"Dynamics and Electrostatics of Membrane Proteins using Polarizable Molecular Dynamics Simulations"*	
Alexa M. Salsbury	Biochemistry	Fall 2017 – Spring 2021
Dissertation:	*"Exploring the Forces Underlying the Dynamics and Energetics of G-quadruplexes with Polarizable Molecular Dynamics Simulations"*	

PH.D. ADVISORY COMMITTEES

Fatemeh Ghafouri	Genetics, Bioinformatics, and Computational Biology	Fall 2024 – Present
Melanie Hempel	Biochemistry	Spring 2021 – Present
Jesse Janoski	Biological Sciences	Fall 2020 – Summer 2023
Kelsie King	Genetics, Bioinformatics, and Computational Biology	Fall 2023 – Present

Sydney Johnson	Biochemistry	Spring 2020 – Spring 2024
Noah Lyons	Biochemistry	Spring 2021 – Spring 2025
Kaitlyn Malewicz (Co-chair)	Biological Sciences	Spring 2020 – Present
Luke Newman	Chemistry	Spring 2023 – Present
Pabina Pokharel	Biochemistry	Spring 2023 – Present
Pierson Rucker	Biochemistry	Spring 2024 – Present
Amanda Sharp	Genetics, Bioinformatics, and Computational Biology	Fall 2020 – Spring 2023

VISITING PH.D. STUDENTS

Ettore Lo Cascio	Università Cattolica del Sacro Cuore (Rome, Italy)	September 2021 – December 2021

M.S. STUDENTS

Alexandra N. Corrigan	Biochemistry	Fall 2019 – Spring 2021
Thesis: *"Electrostatic Properties at the Interface of p53 Transactivation Domain Binding"*		
Sam Farrokhpoor	Biochemistry	Fall 2022 – Spring 2024
Rebekah J. Fogarty	Biochemistry	Fall 2022 – Fall 2024
Thesis: *"Structural Dynamics and Electrostatic Properties of the VEGF and PIM-1 Oncogenic Promoter G-Quadruplexes from Polarizable Molecular Dynamics Simulations"*		
Brian D. Ratnasinghe	Biochemistry	Fall 2019 – Spring 2021
Thesis: *"Polarizable Simulations of the bcl-2 DNA G-Quadruplex and FMRP RNA G-Quadruplex:Duplex Junction Binding Protein"*		

M.S. ADVISORY COMMITTEES

Ryan Antal	Biochemistry	Fall 2019 – Spring 2020
Anthony Briganti	Biochemistry	Summer 2023 – Spring 2024
Taoyi Chen	Chemistry	Spring 2021 – Present
Truitt Elliott	Biochemistry	Fall 2022 – Spring 2023
Elisa Gagliano	Biochemistry	Spring 2019 – Spring 2020
Micah Hoernig	Biochemistry	Spring 2024 – Present
Kelsie King	Biochemistry	Fall 2019 – Spring 2021
Johanna Parsnick	Biochemistry	Spring 2021 – Fall 2021
Spenser Stone	Biochemistry	Spring 2022 – Spring 2023
Nazneen Sultana	Biochemistry	Summer 2018
Amanda Sharp	Biochemistry	Spring 2019 – Spring 2020
Rowan Woolridge	Biochemistry	Fall 2020 – Spring 2022

UNDERGRADUATE RESEARCH STUDENTS

Hemin Chon	Biochemistry	Fall 2017 – Fall 2018
Jason Davidson	Biochemistry (UT-Dallas)	Summer 2021
Tanner J. Dean	Biochemistry	Fall 2018 – Spring 2021
Sam Farrokhpoor	Biochemistry	Summer 2021
Rebekah J. Fogarty	Biochemistry	Summer 2021 – Spring 2022
Patrick Gilles	Computer Science, Biochemistry	Fall 2022 – Present
Zachary Hoyer	Clinical Neuroscience	Spring 2023 – Spring 2024
Jesse R. Janoski	Biochemistry, Biological Sciences	Fall 2017 – Spring 2018
Joshua A. Kraus	Biochemistry, Chemistry	Fall 2018 – Spring 2020
Kelly Luong	Biochemistry	Fall 2017

Candace Miller	Biochemistry	Spring 2023 – Spring 2024
Sienna Morlatt	Biochemistry	Fall 2023 – Spring 2024
Hao Nguyen	Computer Engineering	Spring 2018 – Fall 2018
Nathan Otto	Biochemistry	Summer 2021
Danielle L. Porier	Biochemistry	Fall 2017 – Spring 2018
Brian D. Ratnasinghe	Biochemistry	Fall 2017 – Fall 2019
Igor Soares Canuto	Biochemistry, Systems Biology	Spring 2023
Emily Testa	Biochemistry	Summer 2021
Shelby Waters	Biochemistry	Fall 2021
Karlie M. Wysong	Biochemistry	Spring 2019 – Spring 2020

HIGH SCHOOL STUDENTS

Japjot Singh	Summer 2018
Faraz Zia	Summer 2018
Griffin Yakob	Summer 2023 – Spring 2024