Justin A. Lemkul, Ph.D.

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EDUCATION

May 2012	**Ph.D., Biochemistry** Virginia Polytechnic Institute and State University MILES-IGERT Graduate Certificate
May 2007	**B.S. In Honors, Biochemistry (Summa Cum Laude)** Virginia Polytechnic Institute and State University Minor in Chemistry, Concentration in Biotechnology

EMPLOYMENT AND EXPERIENCE

August 2017 – Present	**Assistant Professor** Department of Biochemistry, Virginia Polytechnic Institute and State University
July 2013 – July 2017	**NIH Ruth L. Kirschstein Postdoctoral Fellow** Department of Pharmaceutical Sciences and Computer-Aided Drug Design Center, University of Maryland, Baltimore
May 2012 – May 2013	**Research Scientist** Department of Biochemistry, Virginia Polytechnic Institute and State University
August 2007 – May 2012	**Graduate Research Assistant** Department of Biochemistry, Virginia Polytechnic Institute and State University

AWARDS AND HONORS

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

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

AFFILIATIONS AND UNIVERSITY SERVICE

2020 – Present	Department of Biochemistry Faculty Senator
2019 – Present	Virginia Tech Division of Systems Biology
2018 – Present	Chapter Advisor, Gamma Iota Chapter of the Alpha Chi Sigma Fraternity
2018 – Present	Virginia Tech Center for Drug Discovery

PEER-REVIEWED PUBLICATIONS (*Corresponding author)

Since starting at Virginia Tech

1. 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.

2. 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)

3. 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)

4. 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)

5. **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)

6. 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.

7. 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)

8. 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.

9. 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.

10. **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.

11. **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)

12. 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.

13. 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)

14. 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.

15. 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

16. 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)

17. 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)

18. **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)

19. **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)

20. **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)

21. **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)

22. 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)

23. **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)

24. 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)

25. 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)

26. **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)

27. **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)

28. **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.

29. 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.

30. **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)

31. 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.

32. 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.

33. **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.

34. **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)

35. **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.

36. **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.

37. **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.

38. **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.

39. 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.

40. **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.

41. **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)

42. 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.

43. **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)

44. **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.

INVITED SEMINARS AND PRESENTATIONS

Since starting at Virginia Tech

1. "Induced Electronic Polarization in RNA G-Quadruplexes and Tetraloop Folding" Telluride Science Research Center. July 2021. (Virtual presentation via Zoom)

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

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

4. "Development of the Drude Polarizable Force Field for DNA and RNA and Applications to Investigations of Nucleic Acid Structure and Dynamics" 259th American Chemical Society National Meeting. Philadelphia, PA, March 2020. (Conference canceled due to COVID-19, delivered online)

5. "Influence of Induced Polarization on the Dynamics and Folding Free Energy of the Amyloid β-Peptide." 259th American Chemical Society National Meeting. Philadelphia, PA, March 2020. (Contributed oral presentation, Conference canceled due to COVID-19, delivered online)

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

7. "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.

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

9. "Insights into DNA and RNA G-Quadruplexes from Polarizable Molecular Dynamics Simulations." 257th American Chemical Society National Meeting. Orlando, FL, April 2019.

Prior to starting at Virginia Tech

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

11. "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.

12. "Influence of Induced Polarization on Amyloid Peptide Misfolding in Different Solution Environments." 249th American Chemical Society National Meeting. Denver, CO, March 2015.

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

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

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

16. "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.

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

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

19. "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** "Nucleic Acid and Amyloidogenic Protein Folding and Dynamics using a Polarizable Force Field Based on the Classical Drude Oscillator Model." 259th American Chemical Society National Meeting. Philadelphia, PA, March 2020. (Poster, Conference canceled due to COVID-19, delivered online)

2. **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)

3. **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")

4. **J.A. Lemkul** and A.D. MacKerell, Jr. "Polarizable Force Field for RNA Based on the Classical Drude Oscillator Model." 254th ACS National Meeting, Washington, DC, August 2017. (Poster)

Prior to starting at Virginia Tech

5. **J.A. Lemkul** and A.D. MacKerell, Jr. "Polarizable Force Field for DNA and RNA Based on the Classical Drude Oscillator Model." 252nd ACS National Meeting, Philadelphia, PA, August 2016. (Poster)

6. **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)

7. **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)

8. **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)

9. **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)

10. **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)

11. **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)

12. **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)

13. **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)

14. **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)

15. **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)

16. **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)

17. **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)

18. **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)

19. **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)

20. **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)

21. **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)

22. **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)

STUDENT AND COLLABORATOR POSTERS AND PUBLISHED PROCEEDINGS

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

1. S. Noskov, S.K. Amin, A. 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)

2. 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.

3. 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.

4. 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.

5. 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)

6. 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)

7. 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.

8. 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")

9. 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.

10. 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.

11. 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.

12. 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.

13. 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.

14. 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.

15. 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.

16. 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.

17. 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.

18. 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.

19. 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.

20. 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.

21. 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.

22. 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.

23. 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.

24. 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

Spring 2021	BCHM 4984 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) 8/1/2019-6/30/2024 2.00 summer
R35GM133754 $1,150,866
Exploring the Role of Electronic Polarization in Biomolecular Folding and Interactions
Role: PI

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

U.S. Department of Energy 9/1/2021-8/30/2023 0.25 summer
$402,774 (Lemkul share: $111,739)
Understanding the Biosynthesis and Functions of Modified F_{430} Coenzymes in Methanogens and Anaerobic Methanotrophs
PI: K.D. Allen Role: Co-PI

COMPLETED GRANT FUNDING

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
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
Nucleic Acids Research
PLoS Computational Biology
PLoS ONE
Proteins: Structure, Function and Bioinformatics
Research on Chemical Intermediates

RSC Advances
Scientific Reports
The Science of Nature (formerly Naturwissenschaften)

GRANT REVIEWER

Defense Threat Reduction Agency (ad hoc, May 2017)
National Fund for Scientific and Technological Development (FONDECYT, Chile) (ad hoc, September 2019)
Partnership for Advanced Computing in Europe (ad hoc, January 2020)

OTHER PROFESSIONAL SERVICE

2021 Co-organizer, "Recent Advances in Molecular Force Fields" symposium, ACS National Meeting

POSTDOCTORAL ASSOCIATES

Marcelo D. Polêto, December 2020 – present
Yue Yu, January 2018 – November 2018 (currently a postdoc at the University of California, Merced)

PH.D. STUDENTS

Darcy S. Davidson	Biochemistry	Fall 2017 – present
Laura I. Gil Pineda	Biochemistry	Spring 2021 – present
Haley M. Michel	Biochemistry	Fall 2020 – present
Julia M. Montgomery	Biochemistry	Fall 2019 – present
Alexa M. Salsbury	Biochemistry	Fall 2017 – Spring 2021

PH.D. ADVISORY COMMITTEES

Patarasuda Chaisupa	Biological Systems Engineering	Spring 2021 – present
Taoyi Chen	Chemistry	Spring 2021 – present
Melanie Hempel	Biochemistry	Spring 2021 – present
Jesse Janoski	Biological Sciences	Fall 2020 – present
Sydney Johnson	Biochemistry	Spring 2020 – present
Noah Lyons	Biochemistry	Spring 2021 – present
Kaitlyn Malewicz	Biological Sciences	Spring 2020 – present
Amanda Sharp	Genetics, Bioinformatics, and Computational Biology	Fall 2020 – present

M.S. STUDENTS

Alexandra N. Corrigan	Biochemistry	Fall 2019 – Spring 2021
Brian D. Ratnasinghe	Biochemistry	Fall 2019 – Spring 2021

M.S. ADVISORY COMMITTEES

Deraldo Andrade	Mining and Minerals Engineering	Fall 2018 – present
Ryan Antal	Biochemistry	Fall 2019 – Spring 2020
Elisa Gagliano	Biochemistry	Spring 2019 – Spring 2020
Kelsie King	Biochemistry	Fall 2019 – Spring 2021

Johanna Parsnick	Biochemistry	Spring 2021 – present
Nazneen Sultana	Biochemistry	Summer 2018
Amanda Sharp	Biochemistry	Spring 2019 – Spring 2020
Rowan Woolridge	Biochemistry	Fall 2020 – present

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 Fogarty	Biochemistry	Summer 2021
Jesse R. Janoski	Biochemistry, Biological Sciences	Fall 2017 – Spring 2018
Joshua A. Kraus	Biochemistry, Chemistry	Fall 2018 – Spring 2020
Kelly Luong	Biochemistry	Fall 2017
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
Emily Testa	Biochemistry	Summer 2021
Karlie M. Wysong	Biochemistry	Spring 2019 – Spring 2020

HIGH SCHOOL STUDENTS

Japjot Singh	Summer 2018
Faraz Zia	Summer 2018