

## Justin A. Lemkul, Ph.D.

---

Department of Biochemistry  
Virginia Tech  
315 Engel Hall  
340 West Campus Dr.  
Blacksburg, VA 24061

Office Phone: (540) 231-3129  
Email: [jalemkul@vt.edu](mailto:jalemkul@vt.edu)  
<http://www.thelemkullab.com>  
<https://orcid.org/0000-0001-6661-8653>  
<http://www.linkedin.com/pub/justin-lemkul/49/404/311>

## 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

---

- 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            1<sup>st</sup> 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            1<sup>st</sup> Place poster (Student Biomedical category), 6<sup>th</sup> 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	Virginia Tech Faculty Senate Operations Officer
2024 – 2025	Ex officio member, Virginia Tech University Council
2023 – 2025	Chair, Virginia Tech Commission on Faculty Affairs
2023 – 2024	Advisor to the Virginia Tech Faculty Senate Cabinet
2023 – 2024	Virginia Tech Faculty Senate Policy and Procedures Committee
2022 – 2025	Virginia Tech Commission on Faculty Affairs
2018 – 2023	Chapter Advisor, Gamma Iota Chapter of the Alpha Chi Sigma Fraternity

## DEPARTMENTAL SERVICE

---

2023 – 2026	Department of Biochemistry Promotion & Tenure Committee
2023 – Present	Biochemistry Graduate Program Director
2022 – 2023	Department of Biochemistry Awards Committee
2022	Department of Biochemistry Communications Committee
2022 – 2023	Department of Biochemistry Search Committee (Department Head)
2021 – 2022	Department of Biochemistry Search Committee (Assistant Professor)
2021 – 2022	Department of Biochemistry Space Committee
2021 – 2022	Department of Biochemistry Promotion & Tenure Committee (non-voting)
2020 – 2026	Department of Biochemistry Faculty Senator
2017 – Present	Department of Biochemistry Graduate Program Committee

## PEER-REVIEWED PUBLICATIONS (\*Corresponding author)

---

### Since starting at Virginia Tech

1. 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.
2. D.S. Davidson and **J.A. Lemkul\*** (2024) "Pyroglutamylation Modulates Electronic Properties and the

- Conformational Ensemble of the Amyloid  $\beta$ -Peptide." *Proteins: Struct, Funct & Bioinf.* In Press. DOI: 10.1002/prot.26677. (NIHMS1966944)
3. 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)
  4. 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)
  5. 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)
  6. 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)
  7. 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  $\beta$ -Peptide" *J. Phys. Chem. B* 126 (39): 7552-7566. (PMC9547858)
  8. 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)
  9. 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)
  10. K.M. King, A.K. Sharp, D.S. Davidson, A.M. Brown,\* and **J.A. Lemkul\*** (2022) "Impact of Electronic Polarization on Preformed,  $\beta$ -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)
  11. M.D. Polêto and **J.A. Lemkul\*** (2022) "TUPÃ: Electric field analyses for molecular simulations" *J. Comput. Chem.* 43 (16): 1113-1119. (PMC9098685)
  12. 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)
  13. 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)
  14. 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)
  15. 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)
  16. 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)
  17. 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)

18. **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)
19. 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.
20. 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)
21. 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.
22. 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.
23. **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.
24. **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)
25. 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.
26. 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)
27. 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.
28. 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**

29. 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)
30. 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)
31. **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)
32. **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)

33. **J.A. Lemkul** and A.D. MacKerell, Jr. (2016) "Balancing Interactions of Mg<sup>2+</sup> 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)
34. **J.A. Lemkul**, S.K. Lakkaraju, and A.D. MacKerell, Jr. (2016) "Characterization of Mg<sup>2+</sup> Distributions around RNA in Solution." *ACS Omega* 1 (4): 680-688. (PMC5088455)
35. 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)
36. **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)
37. 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)
38. 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  $\beta_2$ -adrenergic GPCR." *J. Comput. Chem.* 37 (4): 416-425. (PMC4756637)
39. **J.A. Lemkul**, J. Huang, and A.D. MacKerell, Jr. (2015) "Induced Dipole-Dipole Interactions Influence Unfolding Pathways of Wild-Type and Mutant Amyloid  $\beta$ -Peptides." *J. Phys. Chem. B* 119 (51): 15574-15582. (PMC4690896)
40. **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)
41. **J.A. Lemkul**, S.N. Lewis, J. Bassaganya-Riera, and D.R. Bevan (2015) "Phosphorylation of PPAR $\gamma$  Affects Collective Motions of the PPAR $\gamma$ -RXR $\alpha$ -DNA Complex." *PLoS ONE*. 10 (5): e0123984.
42. 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  $\beta$ -Peptide." *J. Biomol. Struct. Dyn.* 32 (11): 1817-1832.
43. **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)
44. 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.
45. A.M. Brown, **J.A. Lemkul**, N. Schaum, and D.R. Bevan (2014) "Simulations of Monomeric Amyloid  $\beta$ -Peptide (1-40) with Varying Solution Conditions and Oxidation State of Met35: Implications for Aggregation." *Arch. Biochem. Biophys.* 545 (1): 44-62.
46. **J.A. Lemkul** and D.R. Bevan (2013) "Aggregation of Alzheimer's Amyloid  $\beta$ -Peptide in Biological Membranes: A Molecular Dynamics Study." *Biochemistry*. 52 (29): 4971-4980.
47. **J.A. Lemkul\*** and D.R. Bevan (2012) "The Role of Molecular Simulations in the Development of Inhibitors of Amyloid  $\beta$ -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)

48. **J.A. Lemkul** and D.R. Bevan (2012) "Morin Inhibits the Early Stages of Amyloid  $\beta$ -Peptide Aggregation by Altering Tertiary and Quaternary Interactions to Produce 'Off-Pathway' Structures." *Biochemistry*. 51 (30): 5990-6009.
49. **J.A. Lemkul** and D.R. Bevan (2011) "Lipid Composition Influences the Release of Alzheimer's Amyloid  $\beta$ -Peptide from Membranes." *Protein Sci.* 20 (9): 1530-1545.
50. **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.
51. **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.
52. 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.
53. **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.
54. **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)
55. 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.
56. **J.A. Lemkul** and D.R. Bevan (2009) "Perturbation of membranes by the amyloid  $\beta$ -peptide – a molecular dynamics study." *FEBS J.* 276 (11): 3060-3075. (Highlighted in *FEBS J* virtual issue "Protein Misfolding, Prions, and Amyloid," January 2010)
57. **J.A. Lemkul** and D.R. Bevan (2008) "A Comparative Molecular Dynamics Analysis of the Amyloid  $\beta$ -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

---

1. M.D. Polêto, K.D. Allen,\* and **J.A. Lemkul\*** "Structural dynamics of the methyl-coenzyme M reductase active site are influenced by coenzyme F<sub>430</sub> modifications" Revision submitted to *Biochemistry*, BioRxiv DOI: 10.1101/2024.01.07.574536.
2. J.M. Montgomery and **J.A. Lemkul\*** "Quantifying Induced Dipole Effects in Small Molecule Permeation in a Model Phospholipid Bilayer" In Revision for *Journal of Physical Chemistry B*, BioRxiv DOI: 10.1101/2024.03.12.584668.

## INVITED SEMINARS AND PRESENTATIONS

---

### Since starting at Virginia Tech

1. "Electronic Polarization in Nucleic Acids: Implications for Structure, Dynamics, and Drug Design" MoISSI Minisymposium. July 2023.
2. "CHARMM Force Field Development History, Features, and Implementation in GROMACS" BioExcel Webinar Series. November 2021 (Virtual presentation via Zoom)
3. "Induced Electronic Polarization in RNA G-Quadruplexes and Tetraloop Folding" Telluride Science Research Center RNA Dynamics Workshop. July 2021. (Virtual presentation via Zoom)
4. "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)
5. "Dipole-Dipole Interactions Modulate Secondary and Tertiary Structure of Wild-Type and Mutant Amyloid  $\beta$ -Peptides" Spring 2021 American Chemical Society National Meeting. April 2021. (Virtual presentation via Zoom)
6. "Development of the Drude Nucleic Acid Force Field and Applications to G-Quadruplexes" University of Albany. Albany, NY, March 2021. (Virtual presentation via Zoom)
7. "Toward Computational Drug Design Against DNA G-Quadruplexes: Insights from Molecular Dynamics Simulations" Virginia Tech Life Sciences Seminar Series. Blacksburg, VA, October 2020.
8. "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)
9. "Influence of Induced Polarization on the Dynamics and Folding Free Energy of the Amyloid  $\beta$ -Peptide." Spring 2020 American Chemical Society National Meeting. Philadelphia, PA, March 2020. (Contributed oral presentation, Conference canceled due to COVID-19, delivered online)
10. "Properties of DNA and RNA G-Quadruplexes from Polarizable Simulations" Virginia Tech Center for Drug Discovery Annual Workshop. Blacksburg, VA, January 2020.
11. "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.
12. "Drude Polarizable Force Field for Nucleic Acids: Development and Application to G-Quadruplexes" University of Rochester Bioinformatics Cluster Monthly Seminar. Rochester, NY, May 2019.
13. "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

14. "Polarizable Force Field for DNA and RNA Based on the Classical Drude Oscillator Model." Telluride Science Research Center. Telluride, CO, June 2017.
15. "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.
16. "Influence of Induced Polarization on Amyloid Peptide Misfolding in Different Solution Environments." Spring 2015 American Chemical Society National Meeting. Denver, CO, March 2015.
17. "Biomolecular Force Fields: Fundamentals and Improvements for the Next Generation." 8<sup>th</sup> Annual q-bio Summer School, University of New Mexico, Albuquerque, NM, August 2014.

18. "Insights into Protein Complexation and Drug Discovery from Steered Molecular Dynamics Simulations." 2013 GROMACS Workshop and Conference, Charlottesville, VA, September 2013.
19. "Molecular Dynamics Simulations: Using High-Performance Computing to Solve Problems in Biology, Chemistry, and Physics." Roanoke College, Salem, VA, March 2013.
20. "Dimerization of the Amyloid  $\beta$ -Peptide in Biological Membranes." CECAM workshop – Anchoring simulations to experiments: challenges for understanding and treating Alzheimer's disease. Institut de Biologie Physico-Chimique. Paris, France, May 2012.
21. "Advancing Therapeutics for Alzheimer's Disease with Molecular Dynamics Simulations: An Unconventional Approach to Drug Discovery." Washington & Lee University, Lexington, VA, December 2010.
22. "Computational Approaches to Alzheimer's Drug Discovery." University of Virginia, Charlottesville, VA, November 2010.
23. "Advancing Therapeutics for Alzheimer's Disease with Molecular Dynamics Simulations." 2010 meeting of the Virginia Academy of Science (88<sup>th</sup> VAS), James Madison University, Harrisonburg, VA, May 2010.

## POSTERS AND CONFERENCE PRESENTATIONS

---

### Since starting at Virginia Tech

1. **J.A. Lemkul** "Folding and Dynamics of Nucleic Acids: Combining Electronic Polarization, Enhanced Sampling, and Electric Field Calculations" Computational Chemistry Gordon Research Conference, Portland, ME, July 2024.
2. **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.
3. **J.A. Lemkul** "Electric Fields and Induced Polarization Effects in RNA: Implications for Folding and Function" Biophysical Society 68<sup>th</sup> Annual Meeting, Philadelphia, PA, February 2024.
4. **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)
5. **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. Institut de Biologie Physico-Chimique. Paris, France, June 2023. (Oral presentation)
6. **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)
7. **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)
8. **J.A. Lemkul** "Polarizable Molecular Dynamics Simulations of DNA G-Quadruplexes Reveal Different Properties of Nucleobase Electronic Structure and Cation Binding." Biophysical Society 64<sup>th</sup> Annual Meeting, San Diego, CA, February 2020. (Poster)
9. **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")



10. **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**

11. **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)
12. **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. (1<sup>st</sup> Place poster, Pharmaceutical Sciences Postdoc category)
13. **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)
14. **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 59<sup>th</sup> Annual Meeting, Baltimore, MD)
15. **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)
16. **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)
17. **J.A. Lemkul** and D.R. Bevan "Lipid Composition Influences the Release of Alzheimer's Amyloid  $\beta$ -Peptide from Membranes." Spring ICTAS Doctoral Scholars Meeting, Blacksburg, VA, April 2011. (Poster)
18. **J.A. Lemkul** and D.R. Bevan "Ganglioside GM1 Facilitates Release of Alzheimer's A $\beta$  Peptide from Lipid Rafts." ACC Interdisciplinary Forum for Discovery in Life Sciences, Blacksburg, VA, October 2010. (Oral presentation)
19. **J.A. Lemkul** and D.R. Bevan "Ganglioside GM1 Facilitates Release of Alzheimer's A $\beta$  Peptide from Lipid Rafts." 2010 ICTAS Research Day, Blacksburg, VA, September 2010. (Poster)
20. **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 6<sup>th</sup> Annual Research Day, Blacksburg, VA, October 2009. (1<sup>st</sup> Place Student Biomedical poster, oral presentation)
21. **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. 23<sup>rd</sup> Annual Symposium of the Protein Society, Boston, MA, July 2009. (Poster)
22. **J.A. Lemkul** and D.R. Bevan "Dissolving Alzheimer's Amyloid Plaques with Red Wine: Insights from Molecular Dynamics Simulations." 4<sup>th</sup> Annual Virginia Tech Structural Biology Symposium, Blacksburg, VA, March 2009. (Poster)
23. **J.A. Lemkul** and D.R. Bevan "Dissolving Alzheimer's Amyloid Plaques with Red Wine: Insights from Molecular Dynamics Simulations." 25<sup>th</sup> Annual Graduate Student Association Research Symposium, Blacksburg, VA, March 2009. (Poster)
24. **J.A. Lemkul** and D.R. Bevan "Binding of Flavonoids to the Amyloid  $\beta$ -Peptide: Treating Alzheimer's Disease with Red Wine." *Free Radic. Biol. Med.* 45 (1): S87. Suppl. 16<sup>th</sup> Annual Meeting of the Society for Free Radical Biology and Medicine, November 2008. (Poster)

25. **J.A. Lemkul** and D.R. Bevan "Membrane Molecular Dynamics of Alzheimer's Amyloid- $\beta$  Peptide." Dean's Forum on Health, Food, and Nutrition, Blacksburg, VA, November 2007. (Poster)
26. **J.A. Lemkul** and D.R. Bevan "Membrane Molecular Dynamics of Alzheimer's Amyloid- $\beta$  Peptide." 2007 MII Technical Conference and Review, Blacksburg, VA, October 2007. (Poster)
27. **J.A. Lemkul** and D.R. Bevan "A Molecular Dynamics Analysis of the Amyloid- $\beta$  Peptide: Insights into the Molecular Mechanism of Alzheimer's Disease." *Protein Sci.* 16 (S1): 79. 21<sup>st</sup> Annual Symposium of the Protein Society, Boston, MA, July 2007. (Poster and oral presentation)
28. **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 AND PUBLISHED PROCEEDINGS**

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

1. 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.
2. 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.
3. 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.
4. 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.
5. 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.
6. 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" *68<sup>th</sup> Annual Meeting of the Biophysical Society*. Philadelphia, PA.
7. 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" *68<sup>th</sup> Annual Meeting of the Biophysical Society*. Philadelphia, PA.
8. C.J. Miller,\* L.I. Gil Pineda,\*\* and **J.A. Lemkul** (2024) "Characterizing the Electronic Impact of Phosphorylation on GSXS Tetrapeptides" *68<sup>th</sup> Annual Meeting of the Biophysical Society*. Philadelphia, PA.
9. E. Mohammadi\*\* and **J.A. Lemkul** (2024) "Insights into the Electronic and Structural Properties of Cellulose and Amylose: A Comparative Force Field Study" *68<sup>th</sup> Annual Meeting of the Biophysical Society*. Philadelphia, PA.
10. R. Fogarty,\*\* H.M. Michel,\*\* and **J.A. Lemkul** (2024) "Investigating Potential Drug Targets in the *PIM1* Promoter G-Quadruplex" *68<sup>th</sup> Annual Meeting of the Biophysical Society*. Philadelphia, PA.

11. A.M. Goodberlet\*\* and **J.A. Lemkul** (2024) “The Conformational Landscape of A $\beta$ <sub>10-35</sub> from Conventional and Weighted Ensemble Simulations with the Drude Polarizable Force Field” *68<sup>th</sup> Annual Meeting of the Biophysical Society*. Philadelphia, PA.
12. 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” *68<sup>th</sup> Annual Meeting of the Biophysical Society*. Philadelphia, PA.
13. H.M. Michel,\*\* S. Morlatt,\* and **J.A. Lemkul** (2024) “Advancing G-Quadruplex Drug Targeting Through Polarizable Simulations and SILCS” *68<sup>th</sup> Annual Meeting of the Biophysical Society*. Philadelphia, PA.
14. M.D. Polêto and **J.A. Lemkul** (2024) “Optimizing PET biorecycling solutions through electronically polarizable simulations” *68<sup>th</sup> Annual Meeting of the Biophysical Society*. Philadelphia, PA.
15. 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” *68<sup>th</sup> Annual Meeting of the Biophysical Society*. Philadelphia, PA.
16. 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.
17. K. Malewicz,\*\* J.M. Montgomery,\*\* J.W. McGlothlin, and **J.A. Lemkul** (2023) “Using Molecular Dynamics to Connect Genotype to Phenotype” *SMBE23*. Ferrera, Italy.
18. 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.
19. 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)
20. M.D. Polêto and **J.A. Lemkul** (2023) “Active-Site Electronic Properties and Conformational Dynamics of PET-Degrading Enzymes” *67<sup>th</sup> Annual Meeting of the Biophysical Society*. San Diego, CA.
21. L.I. Gil Pineda\*\* and **J.A. Lemkul** (2023) “Using Tetrapeptide GSSS and  $\beta$ -catenin<sup>17-48</sup> to Study the Effects of Phosphoserine on Polypeptide Conformational Ensembles” *67<sup>th</sup> Annual Meeting of the Biophysical Society*. San Diego, CA.
22. 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” *67<sup>th</sup> Annual Meeting of the Biophysical Society*. San Diego, CA.
23. H.M. Michel\*\* and **J.A. Lemkul** (2023) “Determining the Conformational Ensemble of the HIV-1 LTR G-Quadruplexes using Gaussian-Accelerated Molecular Dynamics” *67<sup>th</sup> Annual Meeting of the Biophysical Society*. San Diego, CA.
24. R. Fogarty,\*\* H.M. Michel,\*\* and **J.A. Lemkul** (2023) “Dynamics and Conformational Heterogeneity of the PIM1 G-Quadruplex from Polarizable Molecular Dynamics Simulations” *67<sup>th</sup> Annual Meeting of the Biophysical Society*. San Diego, CA.
25. 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” *G4thuring*, Marienbad, Czech Republic.
26. 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.

27. S. Noskov, S.K. Amin, A.D. MacKerell, D.R. Salahub, and **J.A. Lemkul** (2022) “Drude Polarizable Model of Monovalent Cation-Protein Interactions” *12<sup>th</sup> Triennial Congress of the World Association of Theoretical Chemistry 2022*, Vancouver, Canada. (Contributed oral presentation)
28. 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.
29. M.D. Polêto and **J.A. Lemkul** (2022) “Ion Binding Free-Energy Landscapes for Telomeric and TERRA G-Quadruplexes” *66<sup>th</sup> Annual Meeting of the Biophysical Society*. San Francisco, CA.
30. H.M. Michel\*\* and **J.A. Lemkul** (2022) “A Tale of Two Loops: Polarizable Molecular Dynamics Simulations of Two HIV-1 LTR G-Quadruplexes” *66<sup>th</sup> Annual Meeting of the Biophysical Society*. San Francisco, CA.
31. 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” *66<sup>th</sup> Annual Meeting of the Biophysical Society*. San Francisco, CA.
32. D.S. Davidson\*\* and **J.A. Lemkul** (2022) “Reputation for Aggregation: Effect of Pyroglutamylation on the Amyloid  $\beta$ -Peptide” *66<sup>th</sup> Annual Meeting of the Biophysical Society*. San Francisco, CA. (Platform talk)
33. 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” *66<sup>th</sup> Annual Meeting of the Biophysical Society*. San Francisco, CA. (Platform talk)
34. R. Fogarty,\* H.M. Michel,\*\* S. Farrokhpoor,\* and **J.A. Lemkul** (2022) “Molecular Dynamics Simulations of the Human VEGF Promoter G-Quadruplex” *66<sup>th</sup> Annual Meeting of the Biophysical Society*. San Francisco, CA.
35. 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.
36. 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” *65<sup>th</sup> Annual Meeting of the Biophysical Society*. Virtual.
37. A.N. Corrigan\*\* and **J.A. Lemkul** (2021) “Drude Polarizable Simulations of the p53 Transactivation Domain with Different Binding Partners” *65<sup>th</sup> Annual Meeting of the Biophysical Society*. Virtual.
38. 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  $\beta$ -Peptide” *259<sup>th</sup> American Chemical Society National Meeting*. Philadelphia, PA. (Conference canceled due to COVID-19, delivered online)
39. 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” *259<sup>th</sup> American Chemical Society National Meeting*. Philadelphia, PA. (Conference canceled due to COVID-19, delivered online)
40. 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” *64<sup>th</sup> Annual Meeting of the Biophysical Society*. San Diego, CA.
41. 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  $\beta$ -Peptide” *64<sup>th</sup> Annual Meeting of the Biophysical Society*. San Diego, CA. (Selected for “flash talk”)

42. A.M. Salsbury\*\* and **J.A. Lemkul** (2020) "Influence of Monovalent Cations on the Dynamics of the *c-kit* Promoter G-Quadruplex using Polarizable Molecular Dynamics Simulations" *64<sup>th</sup> Annual Meeting of the Biophysical Society*. San Diego, CA.
43. 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" *64<sup>th</sup> Annual Meeting of the Biophysical Society*. San Diego, CA.
44. 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" *7<sup>th</sup> Annual Virginia Tech Center for Drug Discovery Poster Session*. Blacksburg, VA.
45. 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.
46. 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.
47. 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" *700<sup>th</sup> Section Meeting of the Blue Ridge Section of the American Chemical Society*. Radford, VA.
48. 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.
49. 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" *63<sup>rd</sup> Annual Meeting of the Biophysical Society*. Baltimore, MD.
50. 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" *63<sup>rd</sup> Annual Meeting of the Biophysical Society*. Baltimore, MD.
51. 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" *63<sup>rd</sup> Annual Meeting of the Biophysical Society*. Baltimore, MD.
52. A.M. Salsbury\*\* and **J.A. Lemkul** (2019) "Polarizable Molecular Dynamics Simulations of *c-kit* Oncogene Promoter G-Quadruplexes of Distinct Conformations" *63<sup>rd</sup> Annual Meeting of the Biophysical Society*. Baltimore, MD.
53. 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" *6<sup>th</sup> Annual Virginia Tech Center for Drug Discovery Poster Session*. Blacksburg, VA.
54. 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.
55. 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.
56. 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.

57. 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	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

---

<b>National Institutes of Health (NIGMS)</b> R35GM133754	8/1/2019-6/30/2029 \$2,954,101 cumulative	2.00 summer
---	--	-------------

Exploring the Role of Electronic Polarization in Biomolecular Folding and Interactions  
Role: PI

<b>U.S. Department of Energy</b> DE-SC0022338	9/1/2021-8/30/2023 \$380,000 (Lemkul share: \$69,795)	0.25 summer
--	--	-------------

Understanding the Biosynthesis and Functions of Modified F<sub>430</sub> Coenzymes in Methanogens and Anaerobic Methanotrophs  
Role: Co-PI (K.D. Allen, PI)

<b>National Science Foundation</b> DMR1933525	8/1/2020-7/30/2025 \$22.9M (Lemkul share: \$83,966)	0.25 summer
--	--	-------------

MIP: GlycoMIP – Automating the Synthesis of Rationally Designed Glycopeptides  
Role: Other Senior Personnel (M. Roman, PI)

## COMPLETED GRANT FUNDING

---

<b>Thomas F. and Kate Miller Jeffress Memorial Trust</b>	6/30/2019-8/30/2021 \$120,000	1.41 summer
--	----------------------------------	-------------

Towards Computational Drug Design Against DNA G-Quadruplexes  
Role: PI

<b>National Institutes of Health (NIGMS)</b> F32GM109632	3/1/2014-2/28/2017 \$163,726	12.00 calendar
---	---------------------------------	----------------

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  
Nature Communications  
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

---

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

## EDITORIAL AND OTHER PROFESSIONAL SERVICE

---

2024 Co-Organizer, *Journal of Computational Chemistry* Special Issue in Honor of Alexander MacKerell's 65<sup>th</sup> 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 – present	
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:	<i>"Investigating the Electrostatic Properties and Dynamics of Amyloidogenic Proteins with Polarizable Molecular Dynamics Simulations"</i>	
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
Esmat Mohammadi	Chemical Engineering	Fall 2023 – present
Julia M. Montgomery	Biochemistry	Fall 2019 – Summer 2024
Dissertation:	<i>“Dynamics and Electrostatics of Membrane Proteins using Polarizable Molecular Dynamics Simulations”</i>	
Alexa M. Salsbury	Biochemistry	Fall 2017 – Spring 2021
Dissertation:	<i>“Exploring the Forces Underlying the Dynamics and Energetics of G-quadruplexes with Polarizable Molecular Dynamics Simulations”</i>	

## PH.D. ADVISORY COMMITTEES

---

Taoyi Chen	Chemistry	Spring 2021 – 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 – present
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:	<i>“Electrostatic Properties at the Interface of p53 Transactivation Domain Binding”</i>	
Sam Farrokhpoor	Biochemistry	Fall 2022 – Spring 2024
Rebekah J. Fogarty	Biochemistry	Fall 2022 – Summer 2024
Brian D. Ratnasinghe	Biochemistry	Fall 2019 – Spring 2021
Thesis:	<i>“Polarizable Simulations of the bcl-2 DNA G-Quadruplex and FMRP RNA G-Quadruplex: Duplex Junction Binding Protein”</i>	

## M.S. ADVISORY COMMITTEES

---

Ryan Antal	Biochemistry	Fall 2019 – Spring 2020
Anthony Briganti	Biochemistry	Summer 2023 – Spring 2024
Truitt Elliott	Biochemistry	Fall 2022 – Spring 2023
Elisa Gagliano	Biochemistry	Spring 2019 – Spring 2020
Micah Hoernig	Biochemistry	Spring 2024 –
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