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Assistant Professor, Kansas State University
Department of Anatomy and Physiology
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EDUCATION **PhD Physics** University of Illinois, Urbana, Illinois, USA **2005-08-25 to 2010-08-09**
Thesis: *Nanopore Technology for DNA Sequencing*
BS Physics University of Akron, Akron, Ohio, USA **2001-05-31 to 2005-05-12**
Honors: *summa cum laude*; Minors: Computer Science and Mathematics

RESEARCH AREA **Theoretical and Computational Physiology and Biophysics**
Research Interests: peptide design, molecular dynamics simulations, free-energy calculations, nanomedicine design

PROFESSIONAL EXPERIENCE **Assistant Professor** **2014-09-01 to present**
Kansas State University, Manhattan, Kansas, USA
Department of Anatomy and Physiology, College of Veterinary Medicine

Postdoctoral Researcher **2013-01-23 to 2014-05-28**
CNRS/Université de Lorraine, Nancy, France
Unité Mixte de Recherche 7565, Supervisor: C. Chipot

Postdoctoral Researcher **2011-08-18 to 2012-12-12**
Fraunhofer Chile Research/Universidad Andrés Bello, Santiago, Chile
Center for Bioinformatics and Integrative Biology, Supervisor: F.D. González-Nilo

Postdoctoral Researcher **2010-08-09 to 2011-06-03**
University of Illinois, Urbana, Illinois, USA
Department of Physics, Supervisor: A. Aksimentiev

Research Assistant, University of Illinois, Urbana, Illinois, USA **2006-24-01 to 2010-08-08**
Department of Physics, Advisor: A. Aksimentiev

Research Assistant, University of Akron, Akron, Ohio, USA **2002-05-20 to 2005-05-12**
Department of Physics, Advisor: R. Ramsier

PEER-REVIEWED JOURNAL ARTICLES

* **Boldface** indicates the author was a member of the Comer Research Group when the work was performed.

61. Tse CH, **Comer J**, Chu SKS, Wang Y, Chipot C (2019) Affordable membrane permeability calculations: Permeation of short-chain alcohols through pure-lipid bilayers and a mammalian cell membrane. *J Chem Theory Comput* doi: [10.1021/acs.jctc.9b00022](https://doi.org/10.1021/acs.jctc.9b00022)

60. Liu S, **Comer J**, van Duin ACT, van Duin DM, Liu B, Edgar JH (2019) Predicting the preferred morphology of hexagonal boron nitride domain structure on nickel from ReaxFF-based molecular dynamics simulations. *Nanoscale* 11:5607–5616. doi: [10.1039/C8NR10291K](https://doi.org/10.1039/C8NR10291K)

59. **Azhagiya Singam ER**, Zhang Y, Magnin G, **Miranda-Carvajal I**, **Coates L**, **Thakkar R**, **Poblete H**, **Comer J** (2019) Thermodynamics of adsorption to graphenic surfaces from aqueous solution. *J Chem Theory Comput* 15(2):1302–1316. doi: [10.1021/acs.jctc.8b00830](https://doi.org/10.1021/acs.jctc.8b00830)

58. **Preciado LM**, **Comer J**, Núñez V, Rey-Súarez P, Pereañez J (2018) Inhibition of a snake venom metalloproteinase by the flavonoid myricetin. *Molecules* 23(10):2662. doi: [10.3390/molecules23102662](https://doi.org/10.3390/molecules23102662)

57. **Preciado LM**, Pereañez J, **Azhagiya Singam ER**, **Comer J** (2018) Interactions between triterpenes and a P-I type snake venom metalloproteinase: Molecular simulations and experiments. *Toxins* 10(10):397. doi: [10.3390/toxins10100397](https://doi.org/10.3390/toxins10100397)

56. Wang Y, **Comer J**, Chen Z, Chen J, Gumbart JC (2018) Exploring adsorption of neutral aromatic pollutants onto graphene nanomaterials via molecular dynamics simulations and theoretical linear solvation energy relationships. *Environ Sci Nano* 5:2117–2128. doi: [10.1039/c8en00575c](https://doi.org/10.1039/c8en00575c)

55. Camarada MB, **Comer J**, **Poblete H**, **Azhagiya Singam ER**, Marquez-Miranda V, Morales-Verdejo C, Gonzalez-Nilo FD (2018) Experimental and computational characterization of the interaction between gold nanoparticles and PAMAM dendrimers. *Langmuir* 34(34):10063–10072. doi: [10.1021/acs.langmuir.8b01809](https://doi.org/10.1021/acs.langmuir.8b01809)
54. Thomas SE, **Comer J**, Kim MJ, Marroquin S, Murthy V, Ramani M, Hopke TG, McCall J, Choi SO, DeLong RK (2018) Comparative functional dynamics studies on the enzyme nano-bio interface. *Int J Nanomedicine* 2018(13):4523–4536. doi: [10.2147/IJN.S152222](https://doi.org/10.2147/IJN.S152222)
53. Marasini R, Pitchaimani A, Nguyen TDT, **Comer J**, Aryal S (2018) Influence of polyethylene glycol passivation on the surface plasmon resonance induced photothermal properties of gold nanorods. *Nanoscale* 10:13684–13693. doi: [10.1039/C8NR03026J](https://doi.org/10.1039/C8NR03026J)
52. Tse CH, **Comer J**, Wang Y, Chipot C (2018) Link between membrane composition and permeability to drugs. *J Chem Theory Comput* 14(6):2895–2909. doi: [10.1021/acs.jctc.8b00272](https://doi.org/10.1021/acs.jctc.8b00272)
51. Carrasco-Sánchez V, Marican A, Vergara-Jaque A, Folch-Cano C, **Comer J**, Laurie VF (2018) Polymeric substances for the removal of ochratoxin A from red wine followed by computational modeling of the complexes formed. *Food Chem* 265:159–164. doi: [10.1016/j.foodchem.2018.05.089](https://doi.org/10.1016/j.foodchem.2018.05.089)
50. **Comer J** (2018) Chasing a protein's tail: Detection of polypeptide translocation through nanopores. *Biophys J* 114(4):759–760. doi: [10.1016/j.bpj.2017.12.020](https://doi.org/10.1016/j.bpj.2017.12.020)
49. **Vergara-Jaque A**, Fong P, **Comer J** (2017) Iodide binding in sodium-coupled cotransporters. *J Chem Inf Model* 57(12):3043–3055. doi: [10.1021/acs.jcim.7b00521](https://doi.org/10.1021/acs.jcim.7b00521)
48. Mazloom R, Jaberi-Douraki M, **Comer J**, Volkova V (2017) Potential information loss due to categorization of minimum inhibitory concentration frequency distributions. *Foodborne Pathog Dis* 15(1):44–54. doi: [10.1089/fpd.2017.2301](https://doi.org/10.1089/fpd.2017.2301)
47. Ahumada M, Jacques E, Andronic C, **Comer J**, Poblete H, Alarcon EI (2017) Novel specific peptides as superior surface stabilizers for silver nano structures: Role of peptide chain length. *J Mater Chem B* 5(45):8925–8928. doi: [10.1039/c7tb02349a](https://doi.org/10.1039/c7tb02349a)
46. Alarcon EI, **Poblete H**, Roh H, Couture JF, **Comer J**, Kochevar IE (2017) Rose bengal binding to collagen and tissue photobonding. *ACS Omega* 2(10):6646–6657. doi: [10.1021/acsomega.7b00675](https://doi.org/10.1021/acsomega.7b00675)
45. Calbo J, López-Moreno A, de Juan A, **Comer J**, Ortí E, Pérez EM (2017) Understanding noncovalent interactions of pyrene derivatives with carbon nanotubes. *Chem Eur J* 23:12909–12916. doi: [10.1002/chem.201702756](https://doi.org/10.1002/chem.201702756)
44. **Comer J**, Schulten K, Chipot C (2017) Permeability of a fluid lipid bilayer to short-chain alcohols from first principles. *J Chem Theory Comput* 13(6):2523–2532. doi: [10.1021/acs.jctc.7b00264](https://doi.org/10.1021/acs.jctc.7b00264)
43. **Poblete H**, **Miranda-Carvajal I**, **Comer J** (2017) Determinants of alanine dipeptide conformational equilibria on graphene and hydroxylated derivatives. *J Phys Chem B* 121:3895–3907. doi: [10.1021/acs.jpcc.7b01130](https://doi.org/10.1021/acs.jpcc.7b01130)
42. DeLong RK, Mitchell JA, Morris RT, **Comer J**, Hurst MN, Ghosh K, Wanekaya A, Mudge M, Schaeffer A, Washington LL, Risor-Marhanka A, Thomas S, Marroquin S, Lekey A, Smith JJ, Garrad R, Aryal S, Abdelhakiem M, Glaspell GP (2017) Enzyme and cancer cell selectivity of nanoparticles: inhibition of 3-D metastatic phenotype and experimental melanoma by zinc oxide. *J Biomed Nanotechnol* 13:1–11. doi: [10.1166/jbn.2017.2336](https://doi.org/10.1166/jbn.2017.2336)
41. **Vergara-Jaque A**, **Comer J**, Sepúlveda-Boza S, Santos LS, Mascayano C, Sandoval-Yáñez C (2017) Study of specific interactions in inclusion complexes of amine-terminated PAMAM dendrimer/flavonoids by experimental and computational methods. *Int J Polym Mater* 66(10):485–494. doi: [10.1080/00914037.2016.1252345](https://doi.org/10.1080/00914037.2016.1252345)
40. Chipot C, **Comer J** (2016) Subdiffusion in membrane permeation of small molecules. *Sci Rep* 6:35913. doi: [10.1038/srep35913](https://doi.org/10.1038/srep35913)
39. Márquez-Miranda V, Araya-Durán I, Camarada MB, **Comer J**, Valencia-Gallegos JA, González-Nilo FD (2016) Self-assembly of amphiphilic dendrimers: The role of generation and alkyl chain length in siRNA interaction. *Sci Rep* 6:29436. doi: [10.1038/srep29436](https://doi.org/10.1038/srep29436)

38. Lee C, **Comer J**, Herndon C, Leung N, Pavlova A, Swift R, Tung C, Rowley CN, Amaro R, Chipot C, Wang Y, Gumbart JC (2016) Simulation-based approaches for determining membrane permeability of small compounds. *J Chem Inf Model* 56(4):721–733. doi: [10.1021/acs.jcim.6b00022](https://doi.org/10.1021/acs.jcim.6b00022)
37. **Comer J**, Aksimentiev A (2016) DNA sequence-dependent ionic currents in ultra-small solid-state nanopores. *Nanoscale* 8(18):9600–9613. doi: [10.1039/C6NR01061J](https://doi.org/10.1039/C6NR01061J)
36. **Poblete H**, Agarwal A, Thomas SS, Bohne C, Phospase J, **Comer J**, Alarcon EI (2016) New insights into peptide–silver nanoparticle interaction: Deciphering the role of cysteine and lysine in the peptide sequence. *Langmuir* 32(1):265–273. doi: [10.1021/acs.langmuir.5b03601](https://doi.org/10.1021/acs.langmuir.5b03601)
35. **Comer J**, Chen R, **Poblete H**, **Vergara-Jaque A**, Riviere JE (2015) Predicting adsorption affinities of small molecules on carbon nanotubes using molecular dynamics simulation. *ACS Nano* 9(12):11761–11774. doi: [10.1021/acs.nano.5b03592](https://doi.org/10.1021/acs.nano.5b03592)
34. Fu H, **Comer J**, Cai W, Chipot C (2015) Sonoporation at small and large length scales. effect of cavitation bubble collapse on membranes. *J Phys Chem Lett* 6:413–418. doi: [10.1021/jz502513w](https://doi.org/10.1021/jz502513w)
33. **Poblete H**, Oyarzún I, Olivero P, **Comer J**, Zuñiga M, Sepulveda RV, Báez-Nieto D, Leon CG, González-Nilo F, Latorre R (2015) Molecular determinants of phosphatidylinositol 4,5-bisphosphate (PI(4,5)P₂) binding to transient receptor potential V1 (TRPV1) channels. *J Biol Chem* 290(4):2086–2098. doi: [10.1074/jbc.M114.613620](https://doi.org/10.1074/jbc.M114.613620)
32. Comer J, Gumbart JC, Hénin J, Lelièvre T, Pohorille A, Chipot C (2015) The adaptive biasing force method: everything you always wanted to know but were afraid to ask. *J Phys Chem B* 119(3):1129–1151. doi: [10.1021/jp506633n](https://doi.org/10.1021/jp506633n)
31. Comer J, Phillips JC, Schulten K, Chipot C (2014) Multiple-walker strategies for free-energy calculations in NAMD: Shared adaptive biasing force and walker selection rules. *J Chem Theory Comput* 10(12):5276–5285. doi: [10.1021/ct500874p](https://doi.org/10.1021/ct500874p)
30. Maffeo C, Yoo J, Comer J, Wells DB, Luan B, Aksimentiev A (2014) Close encounters with DNA. *J Phys: Condens Matter* 26(41):413101. doi: [10.1088/0953-8984/26/41/413101](https://doi.org/10.1088/0953-8984/26/41/413101)
29. Comer J, Schulten K, Chipot C (2014) Diffusive models of membrane permeation with explicit orientational freedom. *J Chem Theory Comput* 10(7):2710–2718. doi: [10.1021/ct500209j](https://doi.org/10.1021/ct500209j)
28. Comer J, Schulten K, Chipot C (2014) Calculation of lipid-bilayer permeabilities using an average force. *J Chem Theory Comput* 10(2):554–564. doi: [10.1021/ct400925s](https://doi.org/10.1021/ct400925s)
27. Comer J, Roux B, Chipot C (2014) Achieving ergodic sampling using replica-exchange free-energy calculations. *Mol Sim* 40(1-3):218–228. doi: [10.1080/08927022.2013.841909](https://doi.org/10.1080/08927022.2013.841909)
26. Carrasco-Sánchez V, Vergara-Jaque A, Zuñiga M, Comer J, John A, Nachtigall FM, Valdes O, Duran-Lara EF, Sandoval C, Santos LS (2014) In situ and in silico evaluation of amine- and folate-terminated dendrimers as nanocarriers of anesthetics. *Eur J Med Chem* 73:250–257. doi: [10.1016/j.ejmech.2013.11.040](https://doi.org/10.1016/j.ejmech.2013.11.040)
25. Chaudhry JH, Comer J, Aksimentiev A, Olson LN (2014) A stabilized finite element method for modified Poisson–Nernst–Planck equations to determine ion flow through a nanopore. *Commun Comput Phys* 15:93–125. doi: [10.4208/cicp.101112.100413a](https://doi.org/10.4208/cicp.101112.100413a)
24. Zoonens M, Comer J, Masscheleyn S, Pebay-Peyroula E, Chipot CJ, Miroux B, Dehez F (2013) Dangerous liaisons between detergents and membrane proteins. the case of mitochondrial uncoupling protein 2. *J Am Chem Soc* 135(40):15174–15182. doi: [10.1021/ja407424v](https://doi.org/10.1021/ja407424v)
23. Comer J, Dehez F, Cai W, Chipot C (2013) Water conduction through a peptide nanotube. *J Phys Chem C* 117(50):26797–26803. doi: [10.1021/jp4088223](https://doi.org/10.1021/jp4088223)
22. Vergara-Jaque A, Comer J, Monsalve L, González-Nilo FD, Sandoval C (2013) A computationally efficient methodology for atomic-level characterization of dendrimer–drug complexes: A comparison of amine- and acetyl-terminated PAMAM. *J Phys Chem B* 117(22):6801–6813. doi: [10.1021/jp4000363](https://doi.org/10.1021/jp4000363)
21. Vilos C, Morales FA, Solar PA, Herrera NS, Gonzalez-Nilo FD, Aguayo DA, Mendoza HL, Comer J, Bravo ML, Gonzalez PA, Kato S, Cuello MA, Alonso C, Bravo EJ, Bustamante EI, Owend GI, Velasquez LA (2013) Paclitaxel-PHBV nanoparticles and their toxicity to endometrial and primary ovarian cancer cells. *Biomaterials* 34(16):4098–4108. doi: [10.1016/j.biomaterials.2013.02.034](https://doi.org/10.1016/j.biomaterials.2013.02.034)

20. Comer J, Chipot C, Gonzalez-Nilo FD (2013) Calculating position-dependent diffusivity in biased molecular dynamics simulations. *J Chem Theory Comput* 9(2):876–882. doi: [10.1021/ct300867e](https://doi.org/10.1021/ct300867e)
19. Comer J, Ho A, Aksimentiev A (2012) Toward detection of DNA-bound proteins using solid-state nanopores: insights from computer simulations. *Electrophoresis* 33(23):3466–3479. doi: [10.1002/elps.201200164](https://doi.org/10.1002/elps.201200164)
18. Wells D, Belkin M, Comer J, Aksimentiev A (2012) Assessing graphene nanopores for sequencing DNA. *Nano Lett* 12:4117–4123. doi: [10.1021/nl301655d](https://doi.org/10.1021/nl301655d)
17. Timp W, Comer J, Aksimentiev A (2012) DNA base-calling from a nanopore using a Viterbi algorithm. *Biophys J* 102(10):L37–L39. doi: [10.1016/j.bpj.2012.04.009](https://doi.org/10.1016/j.bpj.2012.04.009)
16. Comer J, Aksimentiev A (2012) Predicting the DNA sequence dependence of nanopore ion current using atomic-resolution Brownian dynamics. *J Phys Chem C* 116(5):3376–3393. doi: [10.1021/jp210641j](https://doi.org/10.1021/jp210641j)
15. Carr R, Comer J, Ginsberg MD, Aksimentiev A (2011) Microscopic perspective on the adsorption isotherm of a heterogeneous surface. *J Phys Chem Lett* 2:1804–1807. doi: [10.1021/jz200749d](https://doi.org/10.1021/jz200749d)
14. Venkatesan B, Polans J, Comer J, Sridhar S, Wendell D, Aksimentiev A, Bashir R (2011) Lipid bilayer coated Al₂O₃ nanopore sensors: towards a hybrid biological solid-state nanopore. *Biomed Microdevices* 13(4):671–682. doi: [10.1021/nl301655d](https://doi.org/10.1021/nl301655d)
13. Carr R, Comer J, Ginsberg M, Aksimentiev A (2011) Atoms-to-microns model for small solute transport through sticky nanochannels. *Lab Chip* 11:3766–3773. doi: [10.1039/C1LC20697D](https://doi.org/10.1039/C1LC20697D)
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10. Timp W, Mirsaidov U, Wang D, Comer J, Aksimentiev A, Timp G (2010) Nanopore sequencing: Electrical measurements of the code of life. *IEEE Tran Nanotechnol* 9(3):281–294. doi: [10.1109/TNANO.2010.2044418](https://doi.org/10.1109/TNANO.2010.2044418)
9. Dorvel B, Sigalov G, Zhao Q, Comer J, Dimitrov V, Mirsaidov U, Aksimentiev A, Timp G (2009) Analyzing the forces binding a restriction endonuclease to DNA using a synthetic nanopore. *Nucl Acids Res* 37:4170–4179. doi: [10.1093/nar/gkp317](https://doi.org/10.1093/nar/gkp317)
8. Aksimentiev A, Brunner R, Cruz-Chu ER, Comer J, Schulten K (2009) Modeling transport through synthetic nanopores. *IEEE Nanotechnol Mag* 3:20–28. doi: [10.1109/MNANO.2008.931112](https://doi.org/10.1109/MNANO.2008.931112)
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6. Sigalov G, Comer J, Timp G, Aksimentiev A (2008) Detection of DNA sequence using an alternating electric field in a nanopore capacitor. *Nano Lett* 8:56–63. doi: [10.1021/nl071890k](https://doi.org/10.1021/nl071890k)
5. Zhao Q, Comer J, Dimitrov V, Aksimentiev A, Timp G (2008) Stretching and unzipping nucleic acid hairpins using a synthetic nanopore. *Nucl Acids Res* 36(5):1532–1541. doi: [10.1093/nar/gkm1017](https://doi.org/10.1093/nar/gkm1017)
4. Farkas N, Comer J, Zhang G, Evans E, Ramsier R, Dagata J (2005) SPM oxidation and parallel writing on zirconium nitride thin films. *J Vac Sci Technol A* 23:846. doi: [10.1116/1.1864052](https://doi.org/10.1116/1.1864052)
3. Farkas N, Comer J, Zhang G, Evans E, Ramsier R, Dagata J (2005) High-voltage SPM oxidation of ZrN: materials for multiscale applications. *Nanotechnology* 16:262–266. doi: [10.1088/0957-4484/16/2/014](https://doi.org/10.1088/0957-4484/16/2/014)
2. Farkas N, Comer J, Zhang G, Evans E, Ramsier R, Wight S, Dagata J (2004) Parallel writing on zirconium nitride thin films by local oxidation nanolithography. *Appl Phys Lett* 85:5691. doi: [10.1063/1.1833569](https://doi.org/10.1063/1.1833569)
1. Comer J, Shepard M, Henriksen P, Ramsier R (2004) Chladni plates revisited. *Am J Phys* 72:1345. doi: [10.1119/1.1758222](https://doi.org/10.1119/1.1758222)

BOOK
CHAPTERS

8. **Poblete H, Comer J** (2019) Computational modeling of the adsorption of capping agent biomolecules to inorganic nanoparticles In *Photoactive Inorganic Nanoparticles*, pages 21–41. Elsevier, Inc. doi: [10.1016/B978-0-12-814531-9.00002-6](https://doi.org/10.1016/B978-0-12-814531-9.00002-6)
7. Carr R, Comer J, Aksimentiev A (2011) Modeling the interface between biological and synthetic components in hybrid nanosystems. In *Simulations in Nanobiotechnology*. CRC Press. ISBN 978-1439835043
6. Wells DB, Bhattacharya S, Carr R, Maffeo C, Ho A, Comer J, Aksimentiev A (2011) Optimization of the molecular dynamics method for simulations of DNA and ion transport through biological nanopores. In *Nanopore-based technology: single molecule characterization and DNA sequencing*. Humana Press. ISBN 978-1-61779-772-9
5. Comer J, Wells DB, Aksimentiev A (2011) Modeling nanopores for sequencing DNA. In *Protocols in DNA nanotechnology*. Humana Press. URL: <http://bionano.physics.illinois.edu/tutorials/modeling-nanopores-sequencing-dna>
4. Comer J, Aksimentiev A (2011) Nanopore force spectroscopy: Insights from molecular dynamics simulations. In *Nanopores: Sensing and Fundamental Biological Interactions*. Springer. ISBN 978-1-4419-8251-3
3. Timp G, Mirsaidov U, Timp W, Shim J, Wang D, Dimitrov V, Scrimgeour J, Lin C, Comer J, Ho HY, Zou X, Aksimentiev A, Schulten K (2011) 3rd generation DNA sequencing with a nanopore. In *Nanopores: Sensing and Fundamental Biological Interactions*. Springer. ISBN 978-1-4419-8251-3
2. Aksimentiev A, Brunner R, Cohen J, Comer J, Cruz-Chu E, Hardy D, Rajan A, Shih A, Sigalov G, Yin Y, Schulten K (2008) Computer modeling in biotechnology: a partner in development. In *Nanostructure Design: Methods and Protocols*, pages 181–234. Humana Press. doi: [10.1007/978-1-59745-480-3_11](https://doi.org/10.1007/978-1-59745-480-3_11) ISBN 978-1-934115-35-0
1. Shepard M, Comer J, Young T, McNatt J, Espe M, Ramsier R, Robinson T, Nelson L (2004) Organophosphate adsorption on metal oxide surfaces. In *Silanes and Other Coupling Agents, Vol. 3*, pages 225–240. VSP: Leiden. ISBN 978-90-67-64404-4

PATENTS

Timp G, Timp W, Mirsaidov U, Aksimentiev A, Comer J (2013) Characterizing Stretched Polynucleotides in a Synthetic Nanopassage *US Patent 8,748,091*

GRANTS

- **K-INBRE Bridging Grant (NIH supported)** 2019-03-01 to 2020-28-02
Role of the intestinal microbiome in anticancer immunity induced by a Euglena water extract
Amount: **\$60,800**. PIs: Masaaki Tamura and Jeffrey Comer
- **Kansas State University CVM SMILE Award** 2018-11-01 to 2019-10-31
Mechanism of anticancer immunity induced by an extract from Euglena gracilis
Amount: **\$32,000**. PI: Masaaki Tamura
- **Johnson Cancer Center Innovative Research Award** 2018-01-01 to 2019-12-31
Cancer-targeted immunotherapy with PD-L1 inhibitory peptide secretory genes and oncolytic virus for the treatment of lung cancer
Amount: **\$20,300**. PI: Masaaki Tamura
- **Euglena Research Contract** 2017-12-01 to 2018-11-30
Evaluation of the effect of Euglena water extract on the growth of lung tumor
Amount: **\$5,987**. PI: Masaaki Tamura
- **NIH NCI R15 (1 R15 CA219919-01)** 2017-08-01 to 2020-07-31
Cancer-targeted local pulmonary immunotherapy with PD-L1 inhibitory peptide secretory genes for the treatment of lung cancer
Direct Costs: **\$250,000**. PIs: Masaaki Tamura and Jeffrey Comer.
- **NSF Major Research Instrumentation (CHE-1726332)** 2017-08-01 to 2020-07-31
MRI: Acquisition of a GPU-enabled computer cluster for molecular modeling applications

Amount: **\$350,000**. PIs: Christine M. Aikens, Bin Liu, Paul E. Smith, Daniel Andresen, Jeffrey Comer.

- Kansas State Global Campus grant 2016-07-01 to 2017-30-06
Development of Computational Comparative Medicine Courses
Award: **\$17,800**. PIs: Ronette Gehring, Jeffrey Comer, Majid Jaber-Douraki, Zhoumeng Lin, Victoriya Volkova.
- XSEDE supercomputer allocation (CHE150078) 2016-01-01 to 2016-12-31
Design of Nanocarriers for Control of Crop Pests
Award: **901,120 service units**, officially valued at \$60,501. PI: Jeffrey Comer.
- Kansas State Global Food Systems grant (383GFS) 2015-05-01 to 2016-04-30
Tapping the Potential of RNA Interference for Agriculture
Award: **\$59,000**. PI: Barry Bradford. Co-PIs: Jeffrey Comer, Glynn Tonsor.
- Pittsburgh Supercomputing Center Anton Allocation (PSCA14057P) 2014-10-20 to 2015-07-31
Bacterial Membrane Selectivity in Antimicrobial Peptides
Award: **50,000 Anton node hours**. PI: Jeffrey Comer.

INVITED
TALKS

- “Optimizing Force Fields for Interactions between Organic Molecules and Nanomaterials Using Experimental Determination of Adsorption Thermodynamics,” CECAM Workshop, Genoa, Italy, to be given 2019-05-30
- “Structure of Proteins at the Surface of Inorganic Materials: An Atomic Perspective,” Center for Computational Biology, University of Kansas, Lawrence, Kansas, 2018-11-13
- “Estructura de proteínas en la superficie de materiales inorgánicos: una perspectiva desde la escala atómica,” *3rd Colombian Conference on Biochemistry and Molecular Biology*, Bogotá, Colombia, 2018-11-03
- “Estructura de proteínas en la superficie de materiales inorgánicos: una perspectiva desde la escala atómica,” *Universidad Antonio Nariño*, Bogotá, Colombia, 2018-11-02
- “Biomolecules at the Water–Nanomaterial Interface: An Atomic-Scale Perspective,” Department of Chemistry, University of West Virginia, Morgantown, West Virginia, 2018-10-17
- “A Molecule’s Eye View of Passive Membrane Permeation: Free Energies and Anomalous Diffusion,” *Membrane Biophysics and Eclipse Symposium*, Manhattan, Kansas, 2017-08-20
- “Adsorción de proteínas a nanomateriales de carbono y su efecto en la estructura de las proteínas,” Universidad Bernardo O’Higgins, Santiago, Chile, 2017-06-16
- “Unpacking the thermodynamics of small solute adsorption on carbon nanomaterials,” *American Chemical Society 51st Midwest Regional Meeting*, Manhattan, Kansas, 2016-10-28
- “Protein Adsorption to Graphene Oxide and Its Effect on Protein Structure,” *Society for Biochemistry and Molecular Biology of Chile: Symposium on Molecular Modeling and Simulation*, Puerto Varas, Chile, 2016-09-29
- “Subdiffusion in Passive Membrane Permeation of Small Molecules,” *Center for the Physics of Living Cells*, University of Illinois, Urbana, Illinois, 2016-09-02
- “Simulations at the Interface between Biology and Synthetic Materials,” *Computational Chemistry Group*, Université de Lorraine, Nancy, France, 2016-06-15
- “Implementing Unusual Force Fields in NAMD,” *NAMD Developer Workshop*, Chicago, Illinois, 2016-05-27
- “Unpacking the Thermodynamics of Small Molecule Adsorption on Nanomaterial Surfaces,” *Mathematical Aspects of Materials Science*, hosted by the Society for Industrial and Applied Mathematics (SIAM), Philadelphia, Pennsylvania, 2016-05-10
- “Molecular Dynamics as a Tool for Nanomaterial Design: Adsorption Affinities of Small Molecules on Carbon Nanotubes and Silver Nanoparticles,” *First International Conference in Bioinformatics, Simulations and Modeling*, Universidad de Talca, Talca, Chile, 2015-11-04
- “Prediction of Adsorption Affinities of Small Molecules on Nanomaterials,” *Free-Energy Calculations. A Mathematical Perspective*, hosted by Banff International Research Station for Mathematical Innovation and Discovery (BIRS), Oaxaca, México, 2015-07-24

- “Fractional kinetics in atomic force microscope assisted oxidation of zirconium nitride,” *Materials Research Society 2004 Fall Meeting*, Boston, Massachusetts, 2004-11-29.

MENTORING	• Ravindra Thakkar, PhD Student	2018-08-20 to present
	• Jocelyn Solorza Márquez, Visiting PhD Student Universidad de Talca, Talca, Chile	2019-02-25 to 2019-05-25
	• E R Azhagiya Singam, Postdoctoral Researcher	2017-08-01 to 2018-08-31
	• Lina María Preciado Rojo, Visiting PhD Student Universidad de Antioquia, Medellín, Colombia	2018-03-26 to 2018-08-18
	• Betty Astrid Velásquez-Silva, Visiting PhD Student Universidad Nacional de Colombia, Bogotá, Colombia	2017-09-18 to 2018-03-17
	• Logan Coates, Undergraduate	2016-09-18 to present
	• Anurag Muthyam, Undergraduate	2016-10-31 to 2017-05-15
	• Horacio Poblete, Postdoctoral Researcher	2015-06-01 to 2017-01-31
	• Ariela Vergara-Jaque, Postdoctoral Researcher	2015-06-01 to 2017-01-31
	• Ingrid Miranda-Carvajal, Visiting PhD Student Universidad Nacional de Colombia, Bogotá, Colombia	2016-08-23 to 2017-02-14
	• Pedro Dousseau Guedes de Melo, Undergraduate	2015-01-19 to 2016-07-22
	• Valeria Márquez-Miranda, Visiting PhD Student Universidad Andrés Bello, Santiago, Chile	2015-05-04 to 2015-07-29

COMER GROUP CONFERENCE ABSTRACTS	• <i>Is the sodium monocarboxylate transporter (SMCT1) a protein involved in the apical iodide transport?</i> Ariela Vergara-Jaque*, Peying Fong, Jeffrey Comer. 60th Annual Biophysical Society Meeting, Los Angeles, California, 2016-02-28
	• <i>New Insight into Peptide-Silver Nanoparticle Interaction: Deciphering the Role of Cysteine and Lysine in the Peptide Sequence</i> , Horacio Poblete*, Anirudh Agarwal, Suma S. Thomas, Cornelia Bohne, Ranjihkumar Ravichandran, Jaywant Phospase, Jeffrey Comer, Emilio I. Alarcon. 60th Annual Biophysical Society Meeting, Los Angeles, California, 2016-02-28
	• <i>Elucidating the Anion Channel Gating Mechanism in Excitatory Amino Acid Transporters</i> , Delany Torres-Salazar*, Horacio Poblete, Aneysis Gonzalez, Ariela Vergara-Jaque, Susan G Amara, Jeffrey Comer. 60th Annual Biophysical Society Meeting, Los Angeles, California, 2016-02-28
	• <i>Mapping Interactions between Nanoparticles and Biomolecules at the Atomic Level</i> , Jeffrey Comer*, Horacio Poblete, Emilio I. Alarcon. 59th Annual Biophysical Society Meeting, Baltimore, Maryland, 2015-02-10
	* presenting author

TEACHING	• Developed and taught graduate course “Structure-Based Drug Design”	Spring 2017, 2019
	• Presented workshop “Fast Free Energy Calculations of Binding to Surfaces”, <i>First International Conference in Bioinformatics, Simulations and Modeling</i> , Universidad de Talca, Talca, Chile, 2015-11-02	
	• Lectures “Nanotechnology in Veterinary Medicine,” 2015-05-07, and “3D Drug Design,” 2016-02-18 and 2017-03-16 for Integration II, Department of Anatomy and Physiology, Kansas State University	
	• Invited lectures for undergrad biophysics courses, Universidad de Talca	2011–2012
	• Guided participants through tutorials at free-energy calc. workshop	Nov. 2011
	• Included in <i>Teachers Ranked as Excellent by Their Students</i>	Fall 2005, Spring 2006
	• Teaching Assistant	
	• Thermal Physics	Fall 2005, Spring 2006, Fall 2006
	• Quantum Physics	Fall 2005, Spring 2006, Fall 2006
	• Music, Sound and Physics (for non-STEM students)	Spring 2004

OUTREACH & TRAINING	• Led computer programming project with gifted program Bergman Elementary, Manhattan, Kansas	2015-01-10 to 2015-05-18
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- Helped expose young people to computer programming through “Hour of Code” hosted by Kansas State’s ACM Chapter, 2014-12-10
- Co-author of molecular simulation tutorials including *Fast Free Energy Calculations of Binding to Surfaces* and *Molecular Modeling of Membrane Proteins: A Homology Modeling Tutorial*, which are freely available at <http://jeffcomer.us/tutorials.html>
- School science demonstrations
 - Lorca Elementary in Chicago, Illinois Jun 2014
 - Escuela Alto Pangué (rural middle school) in San Rafael, Chile Oct 2011
 - Campus Middle School for Girls in Urbana, Illinois Feb 2011

OTHER SKILLS

- Fluency in Spanish, French
- Expertise with molecular dynamics packages: NAMD, LAMMPS, Gromacs, OpenMM
- Knowledge of Rosetta and PyRosetta protein modeling software
- Programming languages: C++ with OpenMP/MPI, CUDA, Tcl/Tk, Bash, HTML/CSS/JavaScript, Matlab/Octave, R, Java, Python
- Contributor to official NAMD source code
- Author of DiffusionFusion software for trajectory analysis:
<https://github.com/jeffcomer?tab=repositories>
- Cover artwork for *The Journal of Physiology* special issue “Twenty-five years of CLC transport proteins” (2015-09-15)