



# Juan Manuel Vanegas, Ph.D.

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## About me

I was born in a small town in the plains of Casanare, Colombia. My brother and I left Colombia when I was 14 years old and came to the United States searching for a better future. With scarce resources, but determined to succeed, I pursued my passion for science to discover how nature works. I am inspired by the microscopic universe of the cell, where billions of molecules come together to propel life.

## Research Interests

Mechanobiology, membrane biophysics, mechanical signal transduction, mechanosensitive channels, multi-scale modeling, classical and *ab initio* molecular simulations, continuum mechanics, materials science, soft condensed matter.

## Education

- Ph.D.** Biophysics. University of California, Davis. **2011**.  
Mentors: Marjorie Longo, Ph.D. and Roland Faller, Ph.D.
- M.S.** Biochemistry and Biophysics. Oregon State University. **2007**
- B.S.** Physics. Oregon State University. **2005**

## Professional Experience

- 2022 –** Associate Professor. Dept. of Biochemistry and Biophysics, Oregon State University.
- 2016 – 22** Assistant Professor. Department of Physics, University of Vermont.
- 2013 – 16** Post-doctoral Researcher. Nanobiology Department, Center for Biological and Materials Sciences. Sandia National Laboratories. Albuquerque, NM. Mentor: Susan B. Rempe, Ph.D.
- 2011 – 13** Post-doctoral Researcher. Department of Applied Mathematics III, Polytechnic University of Catalonia (UPC-BarcelonaTech). Barcelona, Spain. Mentor: Marino Arroyo, Ph.D.

## Grant Proposals

### Awarded

**2020 – 25** “CAREER: Cellular mechanics at the nanoscale: Lipid membrane elasticity and force transduction in mechanosensitive proteins”. Overall budget: **\$635 K for 5 years**. Role: **PI**. NSF grant No. CHE-1944892.

**2019 – 22** “NASA EPSCoR: Novel quantum materials as laboratories for fundamental physics in microgravity”. Overall budget: **\$1.125 M for 3 years**. NASA requested amount: \$750K. UVM cost-sharing: \$375K. Role: **Co-I** with Science-I V. Kotov, and co-Is A. G. Del Maestro, D. Clougherty, T. Lakoba, A. Goodsell, and N. Bigelow. NASA EPSCoR grant No. VT-19-EPSCoR-0010.

**2021 – 23** “An Analog-Independent Synthetic Opioid Detection Technology”. Sub-award budget: **\$46 K for 2 years**. Role: **Co-I** with Co-PIs S.L. Rempe, and M. Moorman. Sandia National Laboratories (DOE).

**2018 – 20** “MRI: Acquisition of a GPU Accelerated Vermont Advanced Computing Core”. Overall budget: **\$1.276 M for 2 years**. NSF requested amount: \$893K. UVM cost-sharing: \$383K. Role: **Co-PI** with PI A. G. Del Maestro, and co-PIs J. Bongard, Y. Chen and H. Garavan. NSF grant No. OAC-1827314.

## Supercomputing Proposals

**2021 – 22** “BIO210065: Mechanical Activation of Membrane Proteins”. Role: **PI**. NSF Extreme Science and Engineering Discovery Environment (XSEDE). Requested hours: **4,454,400 CPU Hrs + 72,800 GPU Hrs** at SDSC Expanse. Pending.

**2019 – 20** “2019AU0117: Mapping the reaction mechanism of bacterial Asparaginases through quantum mechanical calculations”. Role: **PI** with co-I S. B. Rempe. Sandia National Laboratories Center for Integrated Nanotechnologies (CINT) User Proposal.

**2013 – 15** “Fusion of pathogenic viruses studied by molecular dynamics simulations”. Awarded hours: **5,300,000**. Role: **Co-I** with S. B. Rempe. Sandia National Labs.

**2012 – 14** “Role of hopanoids in the mechanical properties of model bacterial membranes and function of mechano-sensitive channels”. Awarded hours: **2,500,000**. Role: **PI** with co-Is M. Arroyo and A. Torres-Sanchez. Barcelona Supercomputing Center.

## Awards and Fellowships

- Biophysical Society Networking Mini-grant to organize the first Green Mountain Molecular Biophysics Symposium at UVM (**2018** and **2019**)
- Biophysical Society Committee on Inclusion and Diversity travel award to attend the 61<sup>st</sup> annual BPS meeting in New Orleans, LA (**2017**)
- International R&D100 Top (Gold) Award Winner in Green Technology for “CO<sub>2</sub> Memzyme,” *R&D Magazine* (**2015**)

- Federal Labs Consortium Award in Notable Technology Development for “Nano-Stabilized Enzymatic Membrane for CO<sub>2</sub> Capture” (**2014**)
- UC Davis George and Dorothy Zolk fellowship (**2010**)
- UC Davis Graduate Research mentorship (**2008**)
- NIH Initiative to Maximize Student Development fellowship (**2007**)
- OSU International Cultural Service Program (ICSP) scholarship (**2003-05**)
- OSU Provost scholarship (**2002-05**)

## Patents

1. Rempe, S. L., Jiang, Y.-B., **Vanegas, J. M.**, Brinker, J. C., and Cecchi, J. L. “Enzymatically active high-flux selectively gas-permeable membranes for enhanced oil recovery and carbon capture.” Application No. US 16/605,466. Pending.
2. Kent, M. S., Rempe, S. L., and **Vanegas, J. M.** “Inhibitors for targeting flaviviruses.” Application No. US 16/684,445. Pending

## Professional Service

- Panel reviewer for NSF Chemical Theory, Models, and Computational Methods (CTMC) (Jan. 21<sup>st</sup> and 22<sup>nd</sup>, 2021)
- Ad-hoc reviewer for NIH Biochemistry and Biophysics of Membranes Study Section (DBIB/BCMB) (Sept. 25<sup>th</sup>, 2019)
- Panel reviewer for Pittsburgh Supercomputing Center “Anton II” proposal allocations organized by the National Academy of Sciences (Sept. 13<sup>th</sup> 2019, Aug. 31<sup>st</sup> 2020, and Sept. 8-10<sup>th</sup> 2021)
- Ad-hoc reviewer for Partnership for Advanced Computing in Europe (PRACE) supercomputing proposal (Jan. 31<sup>st</sup>, 2021)
- Referee for Proc. National Academy of Sciences (PNAS), Nature Chemical Biology, Nature Communications, Journal of Chemical Information and Modeling (ACS), Journal of Chemical Physics (AIP), Journal of Physical Chemistry (ACS), Biomechanics and Modeling in Mechanobiology (Springer), ACS Applied Materials & Interfaces, Langmuir (ACS), Applied Mathematical Modelling (Elsevier), Journal of General Physiology, FEBS Letters

## University and Departmental Service

- Admissions committee for Cellular and Molecular Biosciences (CMB) and Physics Ph.D. graduate programs. Review applications and interview candidates (**2018 - 2021**)
- Physics Dept. Colloquium committee. Invite colloquium speakers and arrange meetings with faculty in the department (**2017** to present)
- Physics Dept. recruitment and outreach activities. Meet with students during visitation days and assist with facility tours (**2017** to present)

- Physics Dept. Active Learning committee (**2016** to present). Meet weekly to discuss implementation of active learning strategies for introductory courses
- UVM College of Arts and Sciences first year student orientation sessions (**2017**)
- Co-organized the first College of Arts and Sciences Vermont Advanced Computing Core User's Meeting with A. del Maestro and J. Li (May 30<sup>th</sup>, **2017**)
- Co-organized the first and second UVM Green Mountain Molecular Biophysics Symposium with J. Li and M. Previs (March 9<sup>th</sup>, **2018** and October 14<sup>th</sup>, **2019**)
- Dissertation committees: Jenna Taft (Chemistry, Ph.D., **2018**), Xing Ke (Materials Science, Ph.D. **2018**), Matthew Luedtke (Chemistry, Ph.D., **2019**), Lily Fang (Materials Science, Ph.D., **2020**), Xiaochuan Zhang (Chemistry, Ph.D., **2020**), Nathan Nichols (Materials Science, Ph.D., **2021**), Kyle McKay (Chemistry, Ph.D., **2021**)

### Professional Affiliations

- American Physical Society
- American Chemical Society
- Biophysical Society

### Teaching Experience

#### *Instructor at UVM*

- **PHYS 011: Elementary Physics**. Algebra-based survey of mechanics, oscillations, waves and thermal physics for students in health and life sciences. Completely re-designed for active learning studio environment. Fall **2019** and Fall **2020**
- **PHYS 096: Extraterrestrial Life**. Newly developed multidisciplinary introductory class exploring the origin of life in the universe and the quest for space exploration. Team taught by faculty in Physics, Geology, English, and Philosophy. Spring **2020** and Spring **2021**
- **PHYS 196: Contemporary Issues in Physics**. Seminar style course covering various topics in differential geometry, elasticity theory, and biophysics. Fall **2018**
- **PHYS 222: Biological Physics**. Newly developed upper division course (undergrad/grad) on the thermodynamics, physics, and mechanics of biological systems. Fall **2016** and Spring **2021**
- **PHYS 256: Introduction to Computational Physics**. Upper division (undergrad/grad) course on computational methods applied to various physics problems (electricity, magnetism, diffusion, etc.). Active learning python-based course with interactive programming activities. Fall **2017**, Fall **2018**, and Fall **2021**
- **PHYS 265: Thermal and Statistical Physics**. Upper division (undergrad/grad) course on thermodynamics and statistical mechanics. Spring **2017**, Spring **2018**, Spring **2019**, and Spring **2020**

- **PHYS 365: Statistical Mechanics.** Upper division (undergrad/grad) course on thermodynamics and statistical mechanics. Fall **2021**

## Mentoring

### *Post-doctoral Associates*

- Dr. Arjun Sharma, Aug. **2020** to present (UVM)
- Dr. Rajitha Rajeshwar Tatikonda, Dec. **2017** to Oct. **2019** (UVM)

### *Graduate Students*

- Andrew Lewis, Physics Ph.D. student, Sept. **2020** to present (UVM)
- Ben Himberg, Materials Science Ph.D. student, June **2017** to present (UVM)
- Bharat Poudel, Materials Science Ph.D. student, Sept. **2017**, to present (UVM)
- Pauline DiGianivittorio, Cellular and Molecular Biosciences Ph.D. student, Aug. **2019** to Nov. **2019** (UVM)
- Alejandro Torres-Sanchez, Applied Mathematics Ph.D. student, **2012 – 2013**, (Polytechnic University of Catalonia)
- Maria Contreras, Bioscience M.S. student, Summer **2010** (UC Davis)

### *Undergraduate Students*

- Patrick Ladd, Physics, May **2021** to present (UVM)
- Ethan Lauricella, Physics, May **2020** to present (UVM)
- Kevin Motia, Physics, Sept. **2020** to June **2021** (UVM)
- Shervin Razavi, Biology and Mathematics, May **2019** to June **2021** (UVM)
- Conner Winkeljohn, Physics, June **2017** to Aug. **2019** (UVM)
- David Peterson, Physics, June **2017** to Dec. **2018** (UVM)
- Renee Beneski, Physics (co-advised with Adrian del Maestro) June **2017** to May **2018** (UVM)
- Clarissa Jordan, Computer Science, Summer **2014**, (Sandia National Laboratories)

## Open Source Projects

- GROMACS-LS – A modified version of the GROMACS molecular simulation package designed for local stress calculations. Main developer with A. Torres-Sanchez [\[Link\]](#)
- MDStressLib – A standalone modular C++ library for local stress calculations from molecular simulations. Main developer with A. Torres-Sanchez [\[Link\]](#)

## Invited Talks and Colloquia

1. **Vanegas, J. M.**, Unravelling the mechanical activation of membrane proteins with MD simulations. Department of Biochemistry and Biophysics, Oregon State

University, Oregon, USA. February 3<sup>rd</sup> **2022**

2. **Vanegas, J. M.**, Under pressure: How mechanical forces “shape” the function of membranes and proteins. Department of Mechanical Engineering, Binghamton University, New York, USA. November 5<sup>th</sup> **2021**

3. **Vanegas, J. M.**, Under pressure: How mechanical forces “shape” the function of membranes and proteins. Center for Computational Biology, University of Kansas, Kansas, USA. November 5<sup>th</sup> **2021**

4. **Vanegas, J. M.**, Under pressure: How mechanical forces “shape” the function of membranes and proteins. Department of Physics Colloquium, Oregon State University, Oregon, USA. May 3<sup>rd</sup> **2021**

5. **Vanegas, J. M.**, Under pressure: How mechanical forces “shape” the function of membranes and proteins. Dept. of Physics and Astronomy Colloquium, University of Delaware, Delaware, USA. March 24<sup>th</sup> **2021**

6. **Vanegas, J. M.**, Microscopic stress in biological membranes: A continuum perspective of MD simulations. Department of Physics. Carnegie Mellon University. Pittsburgh, Pennsylvania, USA. November 5<sup>th</sup> **2019**

7. **Vanegas, J. M.**, Role of chemical structure in the mechanical behavior of biomolecules. Department of Chemistry and Biochemistry. University of Oregon. Eugene, Oregon, USA. October 14<sup>th</sup> **2019**

8. **Vanegas, J. M.**, Feeling the force: Understanding mechanosensation through local stress calculations and steered simulations. Dept. of Chemistry. University of California, Davis, CA, USA. November 13<sup>th</sup> **2018**

9. **Vanegas, J. M.**, Feeling the force: Understanding mechanosensation through local stress calculations and steered simulations. Institute for Physical Science and Technology. University of Maryland, College Park, MD, USA. October 30<sup>th</sup> **2018**

10. **Vanegas, J. M.**, Electronic structure calculations and energetics of L-asparaginase reaction mechanism. Center for Cancer Research, NIH National Cancer Institute. Frederick, Maryland, USA. June 5<sup>th</sup> **2018**

11. **Vanegas, J. M.**, Understanding membrane mechanics and membrane-protein interaction through local stress calculations. Dept. of Physics, Virginia Tech. Apr. 30<sup>th</sup> **2018**

12. **Vanegas, J. M.**, Microscopic stress and nanoscale mechanics of biomolecular systems. Dept. of Physics, Concordia University (Montreal, Canada). Nov. 20<sup>th</sup> **2017**

13. **Vanegas, J. M.**, Microscopic stress and the traction vector in MD simulations. Dept. of Physics and Astronomy, University of Delaware. Sept. 18<sup>th</sup> **2017**

14. **Vanegas, J. M.**, Computational microscopy: Exploring sub-cellular function with molecular modeling. Dept. of Physics, University of Vermont. March 2<sup>nd</sup>, **2016**

### **Workshops/Symposia – Presenter**

1. **Vanegas, J. M.** Locally Distributed Tension MD: A Rapid and Systematic Approach to Study Mechanical Activation of Membrane Proteins. Multiscale

Mechanochemistry and Mechanobiology (Virtual). Organized by the Max Planck Institute for Colloids and Interfaces. August 23-25, **2021**

2. **Vanegas, J. M.**, Calculating Microscopic Elastic Moduli from Atomistic Molecular Dynamics Simulations. Complexity in the Chemistry and Physics of Lipid Membranes (Virtual). Telluride Science Research Center. June 22-25, **2021**

3. **Vanegas, J. M.**, Role of chemical structure in the mechanical behavior of biomolecules. Membranes in Santa Fe Symposium (Organized by the University of Chicago), Santa Fe, New Mexico, USA. June 13<sup>th</sup> **2019**

4. **Vanegas, J. M.**, Molecular and continuum models of elasticity in coiled-coil filamentous proteins. Advanced Materials for Energy and Bioengineering Applications Symposium, University of Vermont. Dec. 4<sup>th</sup> **2017**

5. **Vanegas, J. M.**, Exploring structure, function and mechanics of biomolecules with computer simulations. Advanced Next Generation Energy Leadership Symposium, University of Vermont. Oct. 26<sup>th</sup> **2016**

6. **Vanegas, J. M.**, Is the microscopic stress computed from molecular simulations in mechanical equilibrium? LAMMPS Users' Workshop and Symposium. Albuquerque, New Mexico, USA. (Aug. 5 – 7<sup>th</sup>, **2015**)

### **Workshops/Symposia – Attendee**

1. The Physics of Elastic Films: from Biological Membranes to Extreme Mechanics (Virtual). UC Santa Barbara Kavli Institute for Theoretical Physics. (May 17 – June 18, **2021**)

2. American Association of Physics Teachers new faculty workshop at the American Center of Physics in College Park, MD. (June 12 – 15, **2017**)

3. Short course on multi-scale modeling of materials at the Friedrich-Alexander University in Erlangen, Germany. (February 18 – 22, **2013**)

4. Workshop on numerical methods in applied science and engineering. Barcelona, Spain. (January 21 – 24, **2013**)

5. Entrepreneurship Academy at UC Davis (September 13 – 17, **2010**)

### **Theses**

1. **Vanegas, J. M.** Model yeast biomembranes: Understanding structure and mechanical properties from simulations and experiments. Ph.D. Dissertation. University of California, Davis. (**2011**)

2. **Vanegas, J. M.** Alkylation kinetics of the human retinoid X receptor  $\alpha$  using cysteine as a local probe. Master's Thesis. Oregon State University. (**2007**)

**Publications – Google Scholar *h* – index = 13 (>780 citations) [\[Link\]](#)***Peer-reviewed Journal Articles*

1. **Vanegas, J. M.**, Peterson, D., Lakoba, T., and Kotov, V. N. Spinodal de-wetting of light liquids on graphene. *J. Phys. Condens. Mat.* DOI: 10.1088/1361-648X/ac4f7e (2022) [\[Link\]](#)
2. Del Maestro, A. G., Wexler, C., **Vanegas, J. M.**, Lakoba, T., and Kotov, V. N. A Perspective on Collective Properties of Atoms on 2D Materials. *Adv. Electron. Mater.* 8, 2100607 (2022) [\[Link\]](#)
3. Yu, J., Lauricella, E., Elsayed, M., Shepherd Jr., K., Nichols, N. S., Lombardi, T., Kim, S.-W., Wexler, C., **Vanegas, J. M.**, Lakoba, T., Kotov, V. N., and Del Maestro, A. G. Two-Dimensional Bose-Hubbard Model for Helium on Graphene. *Phys. Rev. B* 103, 235414 (2021) [\[Link\]](#)
4. Rajeswhar Tatikonda, R., Anishkin, A., Sukharev, S., and **Vanegas, J. M.**, Mechanical Activation of MscL Revealed by a Locally Distributed Tension Molecular Dynamics Approach. *Biophys. J.* 120 (2), 232 – 242 (2021) [\[Link\]](#) \*Highlighted under *'New and Notable'* for *Biophys. J.* January issue.
5. Winkeljohn, C. M., Himberg, B., and **Vanegas, J. M.** Balance of Solvent and Chain Interactions Determines the Local Stress State of Simulated Membranes. *J. Phys. Chem. B* 124 (32), 6963 – 6971 (2020) [\[Link\]](#) \*Invited article for virtual special issue *"Computational and Experimental Advances in Biomembranes"*.
6. Lubkowski, J., **Vanegas, J. M.**, Chan, W.-K., Lorenzi, P. L., Weinstein, J. N., Sukharev, S., Fushman, D., Rempe, S. B., Anishkin, A., and Wlodawer, A. The mechanism of catalysis by L-asparaginase. *Biochemistry*, 59, 1927 – 1945 (2020) [\[Link\]](#)
7. Chaudhari, M. I., **Vanegas, J. M.**, Pratt, L. R., Muralidharan, A. and Rempe, S. B. Hydration mimicry by membrane ion channels. *Annu. Rev. Phys. Chem.*, 71, 20.1-20.24 (2020) [\[Link\]](#)
8. Torres-Sanchez, **Vanegas, J. M.**, Purohit, P.K., Arroyo, M. Combined molecular/continuum modeling reveals the role of friction during fast unfolding of coiled-coil proteins. *Soft Matter*, 15, 4961-4975 (2019) [\[Link\]](#)
9. Wen, P.-C., **Vanegas, J. M.**, Rempe, S. B., and Tajkhorshid, E. Probing key elements of teixobactin-lipid II interactions in membrane. *Chem. Sci.* 9, 6997-7008 (2018) [\[Link\]](#)
10. Fu, Y., Jiang, Y., Dunphy, D., Xiong, H., Coker, E., Chou, S., Zhang, H., **Vanegas, J. M.**, Croissant, J., Cecchi, J., Rempe, S. B., and Brinker, C. J. Ultra-thin enzymatic liquid membrane for CO<sub>2</sub> separation and capture. *Nature Commun.* 9 (1), 990 (2018) [\[Link\]](#)
11. **Vanegas, J. M.**, Heinrich, F., Rogers, D. M., Carson, B. D., La Bauve, S., Vernon, B. C., Akgun, B., Satija, S., Zheng, A., Kielian, M., Rempe, S. B., and Kent, M. S. Insertion of dengue E into lipid bilayers studied by neutron reflectivity and molecular dynamics simulations. *Biochim. Biophys. Acta* 1860, 1216–1230 (2018) [\[Link\]](#)



12. Torres-Sanchez, A., **Vanegas, J. M.**, and Arroyo, M. Geometric derivation of the microscopic stress: A covariant central force decomposition. *J. Mech. Phys. Solids* 93, 224 – 239 (2016) [\[Link\]](#)
13. Anishkin, A., **Vanegas, J. M.**, Rogers, D. M., Lorenzi, P. L., Chan, W. K., Purwaha, P., Weinstein, J. N., Sukharev, S., and Rempe, S. B. Catalytic role of the substrate defines specificity of therapeutic L-asparaginase. *J. Mol. Biol.* 427, (17), 2867–2885 (2015) [\[Link\]](#)
14. Torres-Sanchez, A., **Vanegas, J. M.**<sup>\*</sup>, and Arroyo, M. Examining the mechanical equilibrium of microscopic stresses in molecular simulations. *Phys. Rev. Lett.* 114, 258102 (2015). <sup>\*</sup>Co-first author [\[Link\]](#)
15. **Vanegas, J. M.**<sup>\*</sup> and Arroyo, M. Force transduction and lipid binding in Mscl: A continuum-molecular approach. *PLoS ONE*, 9 (12), e113947. (2014). <sup>\*</sup>Corresponding author [\[Link\]](#)
16. **Vanegas, J. M.**, Torres-Sanchez, A., and Arroyo, M. Importance of force decomposition for local stress calculations in biomembrane molecular simulations. *J. Chem. Theory Comput.*, 10, 691-702. (2014) [\[Link\]](#)
17. **Vanegas, J. M.**, Contreras, M. F., Faller, R., and Longo, M. L. Role of unsaturated lipid and ergosterol in ethanol tolerance of model yeast biomembranes. *Biophys. J.*, 102, 507-516. (2012) [\[Link\]](#)
18. **Vanegas, J. M.**, Longo, M. L., and Faller, R. Crystalline, ordered and disordered lipid membranes: Convergence of stress profiles due to ergosterol. *J. Am. Chem. Soc.*, 133, 3720-3723. (2011) [\[Link\]](#)
19. **Vanegas, J. M.**, Faller, R., and Longo, M. L. Influence of ethanol on lipid/sterol membranes: Phase diagram construction from AFM imaging. *Langmuir*, 26, 10415-10418. (2010) [\[Link\]](#)
20. Goksu, I., **Vanegas, J. M.**, Blanchette, C. D., Lin, W-C., and Longo, M. L. AFM for structure and dynamics of biomembranes. *Biochim. Biophys. Acta*, 1788, 254-266. (2009) [\[Link\]](#)

## Poster Presentations

1. Rajeswhar Tatikonda, R., Anishkin, A., Sukharev, S., and **Vanegas, J. M.**, Locally Distributed Tension MD: A Rapid and Systematic Approach to Study Mechanical Activation of Membrane Proteins. 65<sup>th</sup> annual meeting of the Biophysical Society. Virtual. (Feb. 22 – 26, 2021)
2. **Vanegas, J. M.** Lateral Elasticity Profiles of Lipid Membranes from Local Stress Calculations. 64<sup>th</sup> annual meeting of the Biophysical Society. San Diego, California, USA. (Feb. 15 – 19, 2020)
3. Poudel, B., Rajeswhar Tatikonda, R. and **Vanegas, J. M.** Effect of Bilayer Thickness on Mechanical Activation of the Angiotensin II Type 1 Receptor. 64<sup>th</sup> annual meeting of the Biophysical Society. San Diego, California, USA. (Feb. 15 – 19, 2020)
4. Poudel, B., Rajeswhar Tatikonda, R. and **Vanegas, J. M.** Dynamics and

- Energetics of Gating Mechanism in Mechanosensitive Channel of Large Conductance (MscL). 63<sup>rd</sup> annual meeting of the Biophysical Society. Baltimore, Maryland, USA. (March 2 – 6, **2019**)
7. Rajeshwar Tatikonda, R., and **Vanegas, J. M.** Exploring the Hydrophobic Barrier of Human K2P Channel TWIK1 with Steered MD Simulations. 63<sup>rd</sup> annual meeting of the Biophysical Society. Baltimore, Maryland, USA. (March 2 – 6, **2019**)
8. **Vanegas, J. M.**, Winkeljohn, C., and Himberg, B. GROMACS-LS and MDStressLib: Tools for local stress calculations in biomolecular simulations. 63<sup>rd</sup> annual meeting of the Biophysical Society. Baltimore, Maryland, USA. (March 2 – 6, **2019**)
9. Winkeljohn, C., and **Vanegas, J. M.**, Comparison of Atomistic and Coarse-Grain MD Simulations Through Local Stress Analysis of Lipid Bilayers. APS national March meeting. Boston, Massachusetts, USA. (March 4 – 8, **2019**)
10. **Vanegas, J. M.**, Rajeshwar Tatikonda, R. and Arroyo, M. Force transduction and Anchoring of the mechanosensitive channel MscL to lipid membrane through charged interactions. ACS National meeting. Boston, Massachusetts, USA. (August 19 – 23, **2018**)
11. **Vanegas, J. M.**, Winkeljohn, C. M., Torres-Sanchez, A., and Arroyo, M. Mechanics at the nanoscale: Local stress calculations of biomolecular interfaces. 92<sup>nd</sup> ACS Colloids and Surface Science Symposium. State College, Pennsylvania, USA. (June 10 – 13, **2018**)
12. **Vanegas, J. M.**, Himberg, B., and Winkeljohn, C. M. Role of lipid structure in the mechanical properties and stress profiles of lipid biomembranes. APS National March meeting. Los Angeles, California, USA. (March 5 – 9, **2018**)
13. Beneski, R., Del Maestro, A. G., **Vanegas, J. M.**, Kotov, V. Critical films on graphene substrates. APS National March meeting. Los Angeles, California, USA. (March 5 – 9, **2018**)
14. **Vanegas, J. M.**, Torres-Sanchez, A., and Arroyo, M. Beyond lateral pressure profiles: Local stress and the traction vector in MD simulations. Biophysical Society 61<sup>st</sup> annual meeting. New Orleans, Louisiana, USA. (Feb. 11 – 15, **2017**)
15. **Vanegas, J. M.**, Anishkin, A., Rogers, D. M., Sukharev, S., and Rempe, S. B. Active role of the substrate during catalysis by the therapeutic enzyme L-asparaginase II. Biophysical Society 59<sup>th</sup> annual meeting. Baltimore, Maryland, USA. (Feb. 7 – 11, **2015**)
16. **Vanegas, J. M.**, Rogers, D. M., Kent, M. S., and Rempe, S. B. Role of electrostatic interactions in the anchoring of dengue E protein to lipid membranes. Biophysical Society 59<sup>th</sup> annual meeting. Baltimore, Maryland, USA. (Feb. 7 – 11, **2015**)
17. Torres-Sanchez, A., **Vanegas, J. M.**, and Arroyo, M. Local stress calculations: Importance of force decomposition. 11<sup>th</sup> World Congress on Computational Mechanics, Barcelona, Spain. (July 20-25, **2014**)
18. Arroyo, M., Torres-Sanchez, A., **Vanegas, J. M.**, and Rahimi, M. Atomistic and

continuum insights into protein-bilayer interactions. CECAM Workshop on Hybrid Models for Protein-Membrane Interactions, Berlin, Germany. (April 2-4, **2014**)

19. **Vanegas, J. M.** and Arroyo, M. Lipid binding and force transduction in the mechanosensitive channel MscL. Mechanobiology of Proteins and Cells, Biophysical Society meeting. Salisbury Cove, Maine, USA. (Sept. 29 – Oct. 3, **2013**)

20. **Vanegas, J. M.** and Arroyo, M. Role of hopanoids in the mechanics of bacterial membranes and structure of the mechanosensitive channel MscL. Biomembrane Days. Potsdam, Germany. (Sept. 19-21, **2012**)

21. **Vanegas, J. M.** and Arroyo, M. Hopanoids in model bacterial membranes: Structural and mechanical changes in pope bilayers induced by bacteriohopanetetrol. Faraday Discussions 161: Lipids and Membrane Biophysics. London, UK. (Sept. 11-13, **2012**)

22. **Vanegas, J. M.**, Longo, M. L., Faller, R. Ergosterol and temperature modulated changes in dynamic and static properties of DPPC membranes. 241<sup>st</sup> ACS National Meeting, Anaheim, CA, USA. (March 27-31, **2011**)

23. **Vanegas, J. M.**, Block, D. E., Faller, R., Longo, M. L. Microstructural phase changes of DPPC-ergosterol supported membranes stressed by ethanol. APS March National Meeting, Portland, OR, USA. (March 15-19, **2010**)

24. **Vanegas, J. M.**, Longo, M. L., Faller, R. Structure and phase behavior of cholesterol containing membranes in the presence of ethanol. 54<sup>th</sup> Biophysical Society Annual Meeting, San Francisco, CA, USA. (Feb. 20-24, **2010**)

25. **Vanegas, J. M.**, Block, D. E.; Faller, R., Longo, M. L. Effects of temperature on alcohol-induced interdigitation in supported lipid bilayers. 237<sup>th</sup> ACS National Meeting, Salt Lake city, UT, USA. (March 22-26, **2009**)