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

Soft condensed matter physics, multi-scale modeling, molecular simulations (classical and *ab initio*), continuum mechanics, mechanical signal transduction, mechanosensitive channels, ion channels, membrane biophysics.

Education

Ph.D. Biophysics. University of California, Davis. **2011.** Mentors: Dr. Marjorie Longo and Dr. Roland Faller.

M.S. Biochemistry and Biophysics. Oregon State University. **2007**

B.S. Physics. Oregon State University. **2005**

Professional Experience

2016 – Assistant Professor. Dept. of Physics, University of Vermont. Burlington, VT.

2013 – 16 Post-doctoral Researcher. Nanobiology Dept., Center for Biological and Materials Sciences. Sandia National Laboratories. Albuquerque, NM. Mentor: Dr. Susan B. Rempe.

2011 – 13 Post-doctoral Researcher. Dept. of Applied Mathematics III, Technical Univ. of Catalonia (UPC-BarcelonaTech). Barcelona, Spain. Mentor: Dr. Marino Arroyo.

Teaching Experience

Undergraduate

- Biological Physics (PH222). Instructor. UVM, Fall **2016**.

- Properties of Materials. Lab teaching assistant. UC Davis, Winter **2009** and Winter **2011**.
- Molecular and Cellular Biology. Teaching assistant. OSU, Spring **2006**.
- Biochemistry. Teaching assistant. OSU, Fall **2005** and Winter **2006**.
- Scientific Computing I. Teaching assistant. OSU, Fall **2004**.
- Kaplan Inc. MCAT testing preparation instructor, Summer **2003**.
- Mathematics and Computer Science tutor at Umpqua Community college (**2000–02**).

Graduate

- Colloids, Surface Forces and Techniques. Co-Instructor. UC Davis, Spring **2011**.
- Computational Physics I and II. Teaching assistant. OSU, Winter and Spring **2005**.

Professional Service

- Referee for *Journal of Physical Chemistry, Biomechanics and Modeling in Mechanobiology, ACS Applied Materials & Interfaces*.

Professional Affiliations

- Member of *American Physical Society, American Chemical Society, Biophysical Society*.

Mentoring

- Computer Science undergraduate student intern at Sandia (**2014**)
- Physics Ph.D. student at UPC-BarcelonaTech (**2012–13**)
- Bioscience M.S. student intern at UC Davis (**2010**)

Grant Proposals

2015 – 18 "Exploiting the microbial achilles heel for new broad-spectrum anti-microbials". Budget: **$1.5 M for 3 years.** Role: Co-investigator with Principal investigator S. B. Rempe, and co-investigators M. S. Kent, E. Spoerke, and D. Ye. Laboratory Directed Research and Development Proposal 16-0416. Sandia National Laboratories.

Supercomputing Proposals

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

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: **Principal investigator** with co-investigators M. Arroyo and A. Torres-Sanchez. Barcelona Supercomputing Center.

2009 – 11 "A systematic molecular modeling study of the effect of lipid bilayer

composition on resistance to alcohol-induced changes". Awarded Hours: **4,600,000.** Role: Co-investigator with principal investigator R. Faller. Pacific Northwest National Laboratory.

Open Source Projects

- GROMACS-LS – A custom version of the GROMACS molecular simulation package designed for local stress/pressure calculations. Main developer with A. Torres-Sanchez. [Link]
- MDStressLib – A standalone modular C++ library intended for local stress calculations from molecular simulations. Main developer with A. Torres-Sanchez. [Link]

Skills

Computational

- Classical molecular dynamics (GROMACS, NAMD, PLUMED)
- *Ab-initio* electronic structure methods (Gaussian, Q-Chem, VASP)
- Molecular modeling and scientific visualization (UCSF Chimera, VMD, Paraview)
- Python (numpy, scipy, matplotlib)
- Programming (C, C++, bash, java)
- Image processing and analysis (Gwyddion, SimplePCI, ImageJ)
- Parallel computing (MPI)
- Linux/Unix and Linux cluster administration

Laboratory

- Atomic force microscopy
- Fluorescence microscopy
- Basic electron microscopy and 3D image reconstruction
- Preparation of supported membranes and giant unilamellar vesicles
- Protein expression and purification
- Design and creation of custom laboratory equipment
- Liquid chromatography
- SDS-PAGE and electrophoresis
- Absorption, fluorescence, and stopped-flow spectroscopy

Awards and Fellowships

- International R&D100 Top (Gold) Award Winner in Green Technology for "CO_2 Memzyme," *R&D Magazine* (**2015**)
- Federal Labs Consortium Award in Notable Technology Development for "Nano-Stabilized Enzymatic Membrane for CO_2 Capture" (**2014**)

- UC Davis George and Dorothy Zolk fellowship (**2010**)
- UC Davis Graduate Research mentorship (**2008**)
- NIH Initiative to Maximize Student Diversity fellowship (**2007**)
- OSU International Cultural Service Program (ICSP) scholarship (**2003-05**)
- OSU Provost scholarship (**2002-05**)

Special Courses and Workshops

- Short course on multi-scale modeling of materials at the Friedrich-Alexander University in Erlangen, Germany. (February 18 – 22, **2013**)
- Workshop on numerical methods in applied science and engineering. Barcelona, Spain. (January 21 – 24, **2013**)
- Entrepreneurship Academy at UC Davis (September 13 – 17, **2010**)

Publications – Google Scholar *h* – index = 7 (237 citations) [Link]

Peer-reviewed Journal Articles

1. 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]

2. 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]

3. Torres-Sanchez, A., **Vanegas, J. M.***, and Arroyo, M. Examining the mechanical equilibrium of microscopic stresses in molecular simulations. *Phys. Rev. Lett.* 114, 258102 (**2015**). *Co-first author [Link]

4. **Vanegas, J. M.*** and Arroyo, M. Force transduction and lipid binding in MscL: A continuum-molecular approach. *PLoS ONE*, 9 (12), e113947. (**2014**). *Corresponding author [Link]

5. **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]

6. **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]

7. **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]

8. **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]

9. 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]

Manuscripts in Preparation and Under Review

10. Torres-Sanchez, A., Zhao, Q., **Vanegas, J.M.**, Arroyo, M., Purohit, P.K. Progressive unfolding of coiled-coil proteins as a phase transition: A molecular-to-continuum study. *Under review*.

11. **Vanegas, J. M**., Heinrich, F., Akgun, B., Satija, S., Zheng, A., Kielian, M., Carson, B., Rempe, S. B., and Kent, M. S. Insertion of dengue E protein into lipid bilayers resolved by neutron reflectivity and molecular dynamics simulations. *Under review.*

12. Chaudhari, M. I., **Vanegas, J. M.**, and Rempe, S. B. Divalent ion hydration structures and free energies: A step toward assessing hydration mimicry in ion permeation. *In preparation. Invited article at Accounts of Chemical Research.*

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 α using cysteine as a local probe. Master's Thesis. Oregon State University. (2007)

Conference Proceedings and Abstracts

1. **Vanegas, J. M.**, Torres-Sanchez, A., and Arroyo, M. Is the microscopic stress computed from molecular simulations in mechanical equilibrium? LAMMPS Users' Workshop and Symposium. Albuquerque, New Mexico, USA. (Aug. 5 – 7th, **2015**)

2. **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 59th annual meeting. Baltimore, Maryland, USA. (Feb. 7 – 11, **2015**)

3. **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 59th annual meeting. Baltimore, Maryland, USA. (Feb. 7 – 11, **2015**)

4. Torres-Sanchez, A., **Vanegas, J. M.**, and Arroyo, M. Local stress calculations: Importance of force decomposition. 11Th World Congress on Computational Mechanics, Barcelona, Spain. (July 20-25, **2014**)

5. 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**)

6. **Vanegas, J. M.** and Arroyo, M. Lipid binding and force transduction in the

mechanosensitive chanel MscL. Mechanobiology of Proteins and Cells, Biophysical Society meeting. Salisbury Cove, Maine, USA. (Sept. 29 – Oct. 3, **2013**)

7. **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**)

8. **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**)

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

10. **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**)

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

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