

Curriculum Vitae

Jessica MJ Swanson

Assistant Professor
University of Utah, Department of Chemistry

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EDUCATION

University of California at San Diego 2006
PhD in Physical Chemistry; Thesis Advisor: J. Andrew McCammon
Thesis: "Characterizing Biomolecular Recognition and Solvation..."

University of California at Davis 2000
BS in Biochemistry; Research with Alexei Stuchebrukhov
Research: "In silico characterization of cytochrome c oxidase, a redox-driven proton pump"

PROFESSIONAL RESEARCH EXPERIENCE

University of Utah 7/19-present
Assistant Professor

University of Chicago 3/14-6/19
Research Associate Professor
4/10-6/18
Computation Institute Fellow
5/15-3/18
Director of Industrial Relations
7/12-2/14
Research Scientist

Argonne National Laboratory 4/10-4/11
Staff Scientist, Theoretical Chemist

University of Utah, Department of Chemistry 8/09-4/10
Research Assistant Professor
8/06-7/09
Postdoctoral Researcher (NIH NRSA Postdoctoral Fellow)

ADDITIONAL PROFESSIONAL EXPERIENCE

University of Utah 08/20-present
Member of Biological Chemistry Program
11/20-present
Member of Center for Cell and Genome Science
09/20-present
Member of Search Committee for Protein Design Candidate in Biochemistry

University of Chicago 5/12-5/15
Department of Chemistry Industrial Liaison
9/11-8/14
Sustainability Council Member

University of California at San Diego 2005
Established Chancellor's Advisory Committee on Sustainability

- Met with Deans, VP's, and relevant faculty committees gathering support
- Prepared and presented proposal to the UC Board of Regents convincing them to establish an umbrella organization for sustainability

Graduate Student Association Representative & Chair of Sustainable Development Committee 2003-2005

Board of Molecular Biophysics Training Program 2003-2005

<ul style="list-style-type: none"> • Appointed by faculty as only student board member for two years running 	
<i>UCSD Student Sustainability Coalition</i>	2004
<ul style="list-style-type: none"> • Founded/led UCSD branch of grassroots student group (still in existence) 	
<i>Conference Organizer and Chair (Computational Theory Symposium)</i>	2004
<i>Representative for Association of Sci, Biophys, & Molecular Biology (Washington, DC)</i>	2004
<ul style="list-style-type: none"> • Met with 5 House of Representative members advocating science and asking for a strong NIH budget. 	
<i>Coordinator of Biochemistry Seminar Series</i>	2002
<ul style="list-style-type: none"> • Hosted 15 visiting professors taking them to lunch/dinner, orchestrating their schedule, and introducing them at seminars. 	

FELLOWSHIPS

NIH NRSA Ruth L. Kirschstein Postdoctoral Fellow (University of Utah)	2006-2009
ACS PRF Summer School Fellowship (Telluride CO)	2006
Center for Theoretical Biological Physics Fellow (UC San Diego)	2003-2006
Molecular Biophysics Training Grant (UC San Diego)	2002
Gordon-Kenan Chemical Physics Summer School Fellowship (NSF)	2002

AWARDS

ACS Phys. Chem. Postdoctoral Research Highlights, 238 th ACS National Meeting	2009
ACS/CCG Excellence Award, 227 th ACS National Meeting	2004
Exemplary Teaching Assistant Award, UC San Diego	2002
Citation for Outstanding Academic and Research Achievements, UC Davis	2000
Biochemistry Undergraduate Student of the Year, UC Davis	2000
Student's First Achievement Scholarship, UC Davis	1998-1999
Riebsomer Award for Excellence in Chemistry, UNM	1996

INVITED TALKS

Biophysical Dynamics Workshop (Santa Fe, NM)	2020
Co-Organizer of TSRC – Proton Transfer in Biology (Telluride, CO)	2020
Molecular Biophysics of Membranes (Tahoe, CA)	2020
PacifiChem Crossing the Bio Membrane... (Honolulu, HI)	2020
ACS: 3 Symposia	2019
German Biophys Soc: The workings of ion transporters and channels (Berlin, Germany)	2019
Biological Membranes and Membrane Proteins (Santa Fe, NM)	2019
Institute of Biophysical Dynamics Seminar (Chicago, IL)	2019
University of Wisconsin Physical Chemistry Seminar (Madison, WI)	2018
International Symposium on Ion channel design (Gargnano, Italy)	2018
Telluride Science Research Center – Proton Transfer in Biology (Telluride, CO)	2018

Biophysical Society, Membrane Biophysics Subgroup, (San Francisco, CA)	2018
WHO Buruli Ulcer Meeting (Geneva, CH)	2017
Q-Bio Summer School Lecture (Albuquerque, NM)	2014
Telluride Science Research Center - Proton Transfer in Biology (Telluride, CO)	2014
LANL Bioscience Division Colloquium (Los Alamos, NM)	2013
Free Energy Calculations: Three Decades of Adventure in Chemistry (Snowmass, CO)	2013
Genter Symposium: Proton Mobility in Chemical and Bio Systems (Ma`agan Israel)	2010
ACS Special Symposium on Postdoctoral Research Highlights (Washington DC)	2009
Photosynthesis Gordon Research Conference (Smithfield, RI)	2009
American Conference on Theoretical Chemistry (Northwestern, IL)	2008
UC Davis, Department of Chemistry Seminar (Davis, CA)	2005
Telluride Science Research Center - Protein Dynamics (Telluride, CO)	2005
228 th ACS National Meeting, Comp. Division (Philadelphia, PA)	2004
La Jolla Computational Theory Symposium (San Diego, CA)	2004

PUBLICATIONS

1. *How Membrane Curvature and Composition Traffic Amphiphiles*, F Aydin, **JMJ Swanson**, *Proc. Natl. Acad. Sci. USA*, (in preparation).
2. *Improving the accuracy and convergence of drug permeation simulations via machine-learned collective variables*, F Aydin, A Durameric, **JMJ Swanson**, *J. Chem. Theory Comput.*, (in preparation).
3. *Understanding and tracking Protons in Ab Initio Simulations; Insights from IR Spectra*, C Li, GA Voth, **JMJ Swanson**, *J. Phys. Chem. B*, (submitted).
4. *Determinants of Endoplasmic Reticulum-to-Lipid Droplet Protein Targeting*, MJ Olarte, S Kim, ME Sharp, **JMJ Swanson**, RV Farese, TC Walther, *Mol. Cell* (under revision).
5. *Local Conformational Dynamics Regulating Transport Properties of a Cl⁻/H⁺ Antiporter*, Z Wang, **JMJ Swanson**, GA Voth, *J. Comp. Chem.* **41**, 513-519 (2019).
6. *Dynamic Protonation Dramatically Affects the Membrane Permeability of Drug-Like Molecules*, Z Yue, C Li, GA Voth, **JMJ Swanson**, *J. Am. Chem. Soc.* **141** 13421-13433 (2019).
7. *Mycolactone Toxin Membrane Permeation: Atomistic versus Coarse-Grained MARTINI Simulations*, F Aydin, R Sun, **JMJ Swanson**, *Biophys. J.*, **117**, 87-98 (2019).
8. *Proton Induced Conformational and Hydration Dynamics in the Influenza A M2 Channel*, LC Watkins, R Liang, **JMJ Swanson**, WR DeGrado, GA Voth, *J. Am. Chem. Soc.* **141** 11667-11676 (2019).
9. *Multiscale Kinetic Modeling Reveals an Ensemble of Cl⁻/H⁺ Exchange Pathways in ClC-ec1 Antiporter*, HB Mayes, S Lee, GA Voth, **JMJ Swanson**, *J. Am. Chem. Soc.*, **140**, 1793-1804 (2018).
10. *Modulating the Chemical Transport Properties of a Transmembrane Antiporter via Alternative Anion Flux*, Z Wang, **JMJ Swanson**, GA Voth, *J. Am. Chem. Soc.* **140**, 16535-16543 (2018).
11. *Molecular Transport through Membranes: Accurate Permeability Coefficients from Multidimensional Potentials of Mean Force and Local Diffusion Constants*, R Sun, Y Han, **JMJ Swanson**, JS Tan, JP Rose, GA Voth, *J. Chem. Phys.* **149**, 072310-1-11 (2018).

12. *Computational Means of Assessing Proton Pumping in Cytochrome c Oxidase (Complex IV)*, **JMJ Swanson**, chapter in *Mechanisms of Primary Energy Transduction in Biology*, edited by Marten Wikström, Chemical Biology series from Royal Society of Chemistry, (2018).
13. *Membrane Perturbing Properties of Toxin Mycolactone from Mycobacterium Ulcerans*, C Lopez, C Unkefer, BI Swanson, **JMJ Swanson**, S Gnankaran, *PLoS Comput. Biol.*, **14** (2), E1005972-1-22 (2018).
14. *Understanding the Essential Proton Pumping Kinetic Gates and Decoupling Mutations in Cytochrome c Oxidase*, R Liang, GA Voth, M Wikström, **JMJ Swanson**, *Proc. Natl. Acad. Sci. USA*, **114**, 5924-5929 (2017).
15. *Proton Movement and Coupling in the POT Family of Peptide Transporters*, J Parker, C Li, A Brinth, Z Wang, L Vogeley, N Solcan, G Ledderboge-Vucnic, **JMJ Swanson**, M Caffrey, GA Voth, S Newstead, *Proc. Natl. Acad. Sci. USA*, **114** (50), 13182-13187 (2017).
16. *Acid Activation Mechanism of the Influenza A M2 Proton Channel*, R Liang, **JMJ Swanson**, JJ Madsen, M Hong, WF DeGrado, GA Voth, *Proc. Natl. Acad. Sci. USA*, **113** (45), E6955–E6964 (2016).
17. *The Origin of Coupled Chloride and Proton Transport in a Cl⁻/H⁺ Antiporter*, S Lee, HB Mayes, **JMJ Swanson**, GA Voth, *J. Am. Chem. Soc.*, **138**, 14923–14930 (2016).
18. *Coupling Protein Dynamics with Proton Transport in Human Carbonic Anhydrase II*, S Taraphder, CM Maupin, **JMJ Swanson**, GA Voth, *J. Phys. Chem. B*, **120**, 8389–8404 (2016).
19. *Multiscale Simulations Reveal Key Features of the Proton Pumping Mechanism in Cytochrome c Oxidase*, R Liang, **JMJ Swanson**, Y Peng, M Wikström, GA Voth, *Proc. Natl. Acad. Sci. USA*, **113** (27), 7420-7425 (2016).
20. *Multiscale Simulations Reveal Key Aspects of the Proton Transport Mechanism in the ClC-ec1 Antiporter*, S Lee, **JMJ Swanson**, GA Voth, *Biophys. J.*, **110** (6), 1334-1345 (2016).
21. *Computationally Efficient Multiscale Reactive Molecular Dynamics to Describe Amino Acid Deprotonation in Proteins*, S Lee, R Liang, GA Voth, **JMJ Swanson**, *J. Chem. Theory Comput.*, **12** (2), 879-891 (2016).
22. *Hydrated Excess Protons Can Create Their Own Water Wires*, Y Peng, **JMJ Swanson**, S Kang, R Zhou, GA Voth, *J. Phys. Chem. B*, **119** (29), 9212–9218 (2015).
23. *Multiscale Reactive Molecular Dynamics for Absolute pKa Predictions and Amino Acid Deprotonation*, G Nelson, Y Peng, DW Silverstein, **JMJ Swanson**, *J. Chem. Theory Comp.*, **10** (7), 2729-2737 (2014).
24. *Multiscale Simulation Reveals a Multifaceted Mechanism of Proton Permeation through the Influenza A M2 Channel*, R Liang, H Li, **JMJ Swanson**, GA Voth, *Proc. Natl. Acad. Sci. USA* **111** (26), 9396-9401 (2014).
25. *Benchmark Study of the SCC-DFTB Approach for a Biomolecular Proton Channel*, R Liang, **JMJ Swanson**, GA Voth, *J. Chem. Theory Comp.*, **10** (1), 451-462 (2014).
26. *Using Force-Matching to Reveal Essential Differences between Density Functionals in Ab Initio Molecular Dynamics Simulations*, S Izvekov, **JMJ Swanson**, *J. Chem. Phys.*, **134**, 194109-1-14 (2011).
27. *Intricate Role of Water in Proton Transport through Cytochrome c Oxidase*, HJ Lee*, E Svahn*, **JMJ Swanson***, H Lepp, GA Voth, P Brzezinski, GB Gennis, *JACS*, **132** (45), 16225-16239 (2010) (*co-authors contributed equally to this work).
28. *The Role of Charge Transfer in the Structure and Dynamics of the Hydrated Proton*, **JMJ Swanson**, Simons, J, *J. Phys. Chem. B*, **113** (15), 5149-5161 (2009).

29. *Coarse-Graining in Interaction Space*, S Izvekov,* , **JMJ Swanson***, GA Voth, *J. Phys. Chem. B*, **112** (15), 4711-4724 (2008) (*both co-authors contributed equally to this work).
30. *Proton Solvation and Transport in Aqueous and Biomolecular Systems: Insights from Computer Simulations*, **JMJ Swanson**, CM Maupin, H Chen, MK Petersen, J Xu, Y Wu, GA Voth, *J. Phys. Chem. B - Feature Article and Cover*, **111**, 17 (2007).
31. *Optimizing the Poisson-Boltzmann Dielectric Boundary with Explicit Solvent Forces and Energies: Lessons Learned with Atom-Centered Dielectric Functions*, **JMJ Swanson**, JA Wagoner, NA Baker, JA McCammon, *J. Chem. Theory Comput.*, **3**, 170-183 (2007).
32. *Coupling Nonpolar and Polar Solvation Free Energies in Implicit Solvent Models*, J Dzubiella, **JMJ Swanson**, JA McCammon, *J. Chem. Phys.*, **124**, 084905 (2006).
33. *Coupling Hydrophobicity, Dispersion, and Electrostatics in Continuum Solvent Models*, J Dzubiella, **JMJ Swanson**, JA McCammon, *Phys. Rev. Lett.*, **96**, 087802 (2006).
34. *The Entropic Cost of Protein-Protein Association: A Case Study on Acetylcholinesterase Binding to Fasciculin-2*, DDL Minh, JM Bui, CE Chang, T Jain, **JMJ Swanson**, JA McCammon, *Biophys. J.*, **89**, L25-L27 (2005).
35. *Limitations of Atom-Centered Dielectric Functions in Implicit Solvent Models*, **JMJ Swanson**, J Mongan, and JA McCammon, *J. Phys. Chem. B*, **109**, 31, 14769-14772 (2005).
36. *Optimized Radii for Poisson-Boltzmann Calculations with the AMBER Force Field*, **JMJ Swanson**, SA Adcock, and JA McCammon, *J. Chem. Theory Comput.* **3**, 484-493 (2005).
37. *Revisiting Free Energy Calculations: A Theoretical Connection to MM/PBSA and Direct Calculation of the Association Free Energy*, **JMJ Swanson**, RH Henchman, and JA McCammon, *Biophys. J.*, **86**, 67-74 (2004).
38. *Computer Simulation of Water in Cytochrome C Oxidase*, X Zheng, D Medvedev, **J Swanson**, A Stuchebrukhov, *Biochim. Biophys. Acta*, **1557**, 99-107 (2003).