Gianmarc Grazioli, Ph.D.

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Summary

I am an Assistant Professor of Computational Chemistry in the Department of Chemistry at San José State University, where I lead a research group of 2 graduate students and 8 undergraduate students. My research interests lie at the intersection of computational chemistry and biophysics, physical chemistry, chemical physics, data science, machine learning, structural biology, and cheminformatics. My work in these areas has produced 9 peer-reviewed publications, including 6 papers where I am the first author. I aim to leverage my past research experience in developing computational methodologies in enhanced sampling, machine learning, and coarse-grained modeling for molecular systems toward building AI-driven automated discovery methods for the molecular sciences and engineering. I have programming experience in C/C++, R, Mathematica, Python, and Bash, and also have experience with using multiple molecular dynamics software packages, such as NAMD, CHARMM, AMBER, PyMol, and VMD on a variety of high-performance computing clusters. In addition to my academic research experience, I also have industrial experience, both as a member of the management team at the Merck Pharmaceutical Testing Lab for 3 years and as COO/Cofounder of a startup chemical company. Due to my interdisciplinary background, extensive teaching experience, and a full year of graduate pedagogical training, I have strong technical communication skills and am comfortable teaching a wide variety of subject matter.

Education

Ph.D. Chemistry, University of California, Irvine **March 2016**
Advisor: Prof. Ioan Andricioaei
Dissertation title:
"Enhanced Sampling Methods for the Computation of Conformational Kinetics in Macromolecules"

M.S. Chemistry, Villanova University, Villanova, PA **May 2007**
Thesis advisor: Prof. Barry Selinsky
Thesis title: "Structural Requirements for Time-dependent and Time-independent inhibition of Prostaglandin Synthase-1 (COX-1)"

B.S. and B.A. (Comprehensive Science & Science Communication, respectively) **January 2005**
Villanova University, Villanova, PA

Academic Appointments

Assistant Professor of Computational Chemistry, San José State University **July 2020 – present**
Department of Chemistry

Postdoctoral Researcher, University of California, Irvine **April 2017 – April 2020**
Advised jointly by Prof. Carter T. Butts and Prof. Rachel W. Martin
California Institute for Telecommunications and Information Technology (Calit2)
Department of Chemistry

Postdoctoral Researcher, University of California, San Diego **March 2016 - March 2017**
Advisor: Prof. Francesco Paesani
Department of Chemistry and Biochemistry

Publications

Yu, Y.; **Grazioli, G**.; Unhelkar, M.H.; Martin, R.W.; Butts, C.T.; Network Hamiltonian models reveal pathways to amyloid fibril formation. *Scientific reports* 10.1 1-11 (2020): *https://www.nature.com/articles/s41598-020-72260-8*

Grazioli, G.; Yu, Y.; Unhelkar, M.H.; Martin, R.W.; Butts, C.T.; Network-based Classification and Modeling of Amyloid Fibrils. *Journal of Physical Chemistry (ACS) (2019)* *https://pubs.acs.org/doi/abs/10.1021/acs.jpcb.9b03494*

Grazioli, G.; Roy, S.; Butts, C.T.; Predicting Reaction Products and Automating Reactive Trajectory Characterization in Molecular Simulations with Support Vector Machines. *Journal of Chemical Information and Modeling (ACS) (2019)* *https://pubs.acs.org/doi/abs/10.1021/acs.jcim.9b00134*

Grazioli, G.; Martin, R.W.; Butts, C.T.; Comparative Exploratory Analysis of Intrinsically Disordered Protein Dynamics using Machine Learning and Network Analytic Methods. *Frontiers in Molecular Biosciences (2019)* *https://doi.org/10.3389/fmolb.2019.00042*

Grazioli, G.; Andricioaei, I. Advances in Milestoning I: Enhanced Sampling via wind-assisted reweighted milestoning (WARM). *Journal of Chemical Physics* 149.8 (2018): 084103. https://aip.scitation.org/doi/abs/10.1063/1.5029954

Grazioli, G.; Andricioaei, I. Advances in Milestoning II: Calculating time-correlation functions from milestoning using stochastic path integrals. *Journal of Chemical Physics* 149.8 (2018): 084104. https://aip.scitation.org/doi/abs/10.1063/1.5037482

Grazioli, G.; Butts, C.; Andricioaei, I. Automated Placement of Interfaces in Conformational Kinetics Calculations Using Machine Learning, *Journal of Chemical Physics* 147.15 (2017): 152727. http://aip.scitation.org/doi/abs/10.1063/1.4989857

Zhou, H.; Kimsey, I.J.; Nikolova,E.N.; Sathyamoorthy,B.; **Grazioli, G**.; McSally,J.; Bai,T., et al. m1A and m1G disrupt A-RNA structure through the intrinsic instability of Hoogsteen base pairs. *Nature Structural & Molecular Biology* 23.9 (2016): 803. http://www.nature.com/nsmb/journal/v23/n9/full/nsmb.3270.html

Roy, M.; **Grazioli, G**. ; Andricioaei, I. Rate turnover in mechano-catalytical coupling: A model and its microscopic origin, *Journal of Chemical Physics* 143.4 (2015): 07B617_1. http://scitation.aip.org/content/aip/journal/jcp/143/4/10.1063/1.4926664

Manuscript under Review

Yu, Y.; **Grazioli, G**.; Phillips, N.E.; Butts, C.T.; Local Graph Stability in Exponential Family Random Graph Models. ***Revise and Resubmit*** at *Society for Industrial & Applied Mathematics (SIAM) - Journal on Discrete Mathematics.* Preprint available on arXiv: https://arxiv.org/abs/1908.09470

Conference Presentations

Grazioli, G.; Yu, Yue; Unhelkar, M.H.; Martin, R.W.; Butts, C.T.;. Algorithms for parameterizing network Hamiltonians for simulation of amyloid fibril self-assembly. Poster presentation, Biophysical Society Conference (Fall 2020)

Grazioli, G.; Roy, Saswata.; Butts, C.T.;. ML models that both learn and teach chemistry via partitioning reactive trajectories by reaction product in phase space using support vector machines. Oral presentation, American Chemical Society National Conference (Fall 2019)

Grazioli, G.; Yu, Y.; Unhelkar, M.H.; Martin, R.W.; Butts, C.T.;. Topological coarse-graining: Building ultra efficient computer models of aggregation using network Hamiltonians. Oral presentation, American Chemical Society National Conference (Fall 2019)

Grazioli, G.; Roy, Saswata.; Butts, C.T.;. ML models that both learn and teach chemistry via partitioning reactive trajectories by reaction product in phase space using support vector machines. Poster presentation selected for Sci Mix American Chemical Society National Conference (Fall 2019)

Grazioli, G.; Yu, Y..; Butts, C.T.;. Geometric approach toward identifying stable parameters for network Hamiltonians governing amyloid fibril formation. Poster presentation, American Chemical Society National Conference (Fall 2019)

Grazioli, G.; Yu, Y.; Unhelkar, M.H.; Martin, R.W.; Butts, C.T.;. Network Hamiltonians for Modeling Amyloid Fibril Formation. Poster Presentation SoCal Theoretical Chemistry Conf. (2019)

Grazioli, G.; Yu, Y.; Unhelkar, M.H.; Martin, R.W.; Butts, C.T.;. Network-based Modeling of Amyloid Fibril Formation. Poster presentation at Biophysical Society annual meeting (2019)

Unhelkar, Megha H.; Duong, V.T.; **Grazioli, G**.; Kelly, J.E.; Yu, Y.; Butts, C.T.; Martin, R.W.; Leveraging molecular modeling, experimental chemistry and bioinformatics techniques to discover and characterize novel proteins. Poster Presentation at Biophysical Society annual meeting (2020)

Unhelkar, Megha H.; Duong, V.T.; **Grazioli, G**.; Kelly, J.E.; Yu, Y.; Butts, C.T.; Martin, R.W.; Protein Discovery and Characterization Using Molecular Modeling, Experimental Chemistry, and Bioinformatics. Poster Presentation at Biophysical Society annual meeting (2019)

Grazioli, G.; Andricioaei, I.; & Butts, Carter T.; Using machine learning to automate calculations of conformational kinetics in molecular simulations. Oral presentation, American Chemical Society annual meeting, New Orleans, LA. (2018).

Grazioli, G. From Chemists Know to Shredded Science: Using accessible online outreach videos to ignite interest in and aid understanding of chemical concepts. Oral presentation, American Chemical Society annual meeting, San Francisco (2017).

Grazioli, G. & Andricioaei, I. Advancements in Milestoning: 1) Computational speedup by re-weighting artificially accelerated trajectories, and 2) Venturing into the non-equilibrium with coarse-grained random walks in Milestone**,** Oral presentation, American Chemical Society meeting, San Diego, CA. (2016).

Grazioli, G. & Andricioaei, I. Calculating Watson-Crick to Hoogsteen Transition Kinetics in DNA with Langevin Dynamics and Fokker-Planck Diffusion in Reduced Configuration Space**,** Poster presentation, Biophysical Society annual meeting, Los Angeles, CA. (2016).

Grazioli, G. & Andricioaei, I. A Smoluchowski Equation for Force-Modulated Chemistry in Single Molecule Pulling Experiments**.** Poster presentation, Biophysical Society annual meeting, Baltimore, MD. (2015).

Grazioli, G.; Butts, C., & Andricioaei, I. Conformation Space Graphs of Macromolecules: From Network Inference to Dynamics**,** Poster presentation, UCI Data Science Initiative (2015)

Grazioli Johns, G., Conway, A., & Selinsky, B. Structural Requirements for Time-Dependent and Time-Independent Inhibition of Prostaglandin Synthase I (COX I). Poster, American Chemical Society national meeting, San Francisco (2006)

Honors and Awards

- Presentation "ML models that both learn and teach chemistry via partitioning reactive trajectories by reaction product in phase space using support vector machines." selected for Sci Mix American Chemical Society National Conference (Fall 2019)
- Journal of Chemical Physics 2018 Editor's Pick for article titled "Advances in Milestoning II: Calculating time-correlation functions from milestoning using stochastic path integrals"
- Journal of Chemical Physics 2015 Editor's Choice Award for publication entitled "Rate turnover in mechano-catalytic coupling: A model and its microscopic origin"
- University of California, Irvine Data Science Initiative Summer Fellowship, 2015
- Acceptance with Full Scholarship to the Telluride School on Theoretical Chemistry (2015)
- University of California Regent's Dissertation Fellowship, 2015
- University of California, Irvine Pedagogical Fellow, 2014-2015 (included a full year of graduate coursework in advanced pedagogy/student-centered active learning, and design and implementation of TA training for two incoming cohorts of chemistry graduate students)

- UCI School of Physical Sciences fellowship for the development of chemistry educational outreach videos for teaching thermodynamics, "Shredded Science" pilot www.youtube.com/shreddedscience as a follow up to the "Chemists Know" music video (https://youtu.be/iM_I6rtIgn0) (over 464,000 views)

Teaching Experience

Assistant Professor of Computational Chemistry, San José State University……present
Mathematics Professor for STOVS (Pre-college summer bridge program), Villanova University…….2016
Mathematics Teaching Assistant for STOVS, Villanova University……..2011, 2014, 2015
Graduate Teaching Assistant, University of California, Irvine…….2011-2016

- Undergraduate Physical Chemistry (parts I, II, and III), Computational Chemistry Lab, Graduate Thermodynamics and Intro to Statistical Mechanics, & Analytical Chemistry Lab

Part-Time Lecturer, University of Colorado, Boulder…….2010

- General Chemistry, Honors General Chemistry, General Chemistry for Engineers

Graduate Teaching Assistant, Villanova University……..2006-2007

- General Chemistry and Organic Chemistry

High School Physics Teacher, Bethlehem Catholic High School, Bethlehem, PA……...2002-2003
Guitar Instructor, Music Learning Center Rosemont, PA……...2004-2005

Industry and Entrepreneurial Experience

Data Analyst, Pharmaceutical Testing Lab, Merck and Co, West Point, PA 2007-2010

- 3 years of management experience in the pharmaceutical industry at the Merck Pharmaceutical Testing Lab (analytical chemistry cGMP laboratory setting). Was a member of the management team that supervised over 30 chemists who performed analytical testing of finished drugs, and both drug and vaccine raw materials. (Methods: LC, GC, IR, UV/Vis, KF, pH, ICP-AA, IC)

Chief Operations Officer & Cofounder, Emerson Scientific (chemical startup), Los Angeles, CA 2017-2018

- Emerson Scientific was a startup chemical company focused on the development of commercial applications for Nobel Laureate Barry Sharpless's research in Sulfur (VI) Fluoride (SuFEx) "click" chemistry. Responsibilities included serving as liaison between the scientists at Scripps and business development unit, identification of high market value industrial applications for SuFEx, identification of and pitching to potential investors, communicating scientific findings and market potential to potential investors, and the preparation of business plans, pitch decks, and other business documents.

Invited Talks

- SJSU Chemistry Departmental Seminar: "Augmented Chemical Intuition: Computational Methods for Exploring Chemistry with Simulation and Artificial Intelligence" Fall 2020
- UCI Molecular Dynamics Seminar talk, "Molecular Simulation Methods for Traversing Barriers in Time and Complexity" (2018)
- Seminar Speaker for UC Irvine Structural and Chemical Biology Club (2018)
- Guest lecturer: Prof. David Olsen (Cal State Los Angeles) (2018), Communicating Science
- Guest lecturer: Prof. Craig Martens (UCI) (2017) Undergraduate Thermodynamics
- Guest lecturer: for Professor R. Penner (UCI) (CHM 131C: Thermodynamics & Chemical Dynamics, 2012); Professor R. Martin (UCI) (CHM 131B: Molecular Structure & Statistical Mechanics, 2013); Professor C. Martens (UCI) (CHM 131C: Thermodynamics & Chemical Dynamics, 2013)
- UCI Molecular Dynamics Seminar talk, "Accelerated Computation of Timescales for Complex Processes Using "Wind" Assisted Reweighted Milestoning" (2014)
- Invited panelist: UCI Teaching Learning, & Technology Center (2015)

Service and Outreach

- I have generated over 1 million total views on YouTube with my various educational content
- I served on the Chemistry Curriculum Committee Fall 2020
- Served as a reviewer for the Journal of Chemical Physics Summer 2020
- Senior Trainer for the UCI Teaching Assistant Professional Development Program, Fall 2015
- Trainer for the Teaching Assistant Professional Development Program Fall 2014, UCI (both developed and implemented TA training as part of my UCI Pedagogical Fellowship)
- Co-created the "Chemists Know" (https://youtu.be/iM_I6rtIgn0) outreach music video on YouTube (over 439,000 views) with the UC Irvine Chemistry Dept. I wrote, performed, and recorded the song parody, and also played the lead role in the music video.
- Co-creator/writer/host of "Shredded Science" (www.youtube.com/shreddedscience), an ambitious web series on YouTube, that teaches mathematically challenging concepts in science using song parodies, demonstrations, props, computer simulations, and humor (think Weird Al meets Bill Nye). The first episode explains the 1st, 2nd, and 3rd law of thermodynamics using both a song parody I wrote and performed, titled "Thermodynamics (The Macro World)" (https://youtu.be/H1AeVa9FhLY) along with three demonstration/lecture videos I wrote and delivered (e.g. 2nd Law: https://youtu.be/a3kxwYDnKMM).
- Live performance of "Chemists Know" and research talk "Chemistry Rocks" at Cal State Los Angeles for ACS National Chemistry Week.
- Live performance of "Chemists Know" and "Thermodynamics (The Macro World)" on the main stage of the Los Angeles March for Science
- Live performance of "Chemists Know" at California You Be The Chemist state academic competition
- Volunteer for organizing the 1st Southern California Theoretical Chemistry Conference, 2016
- STEM Advisor for STOVS summer bridge program, Villanova University 2018
- Mathematics Professor for STOVS summer bridge program, Villanova University, 2016
- Senior Trainer for the UCI Teaching Assistant Professional Development Program, Fall 2015
- Served as senior graduate student mentor for 1st year graduate student at UCI, 2015
- Career panel member for STOVS summer bridge program, Villanova University, 2015
- Career Day speaker at Allesandro Elementary School, Echo Park, Los Angeles, CA, 2015
- Educational Outreach at STEMploration, Santa Ana, CA, 2015
- Trainer for the Teaching Assistant Professional Development Program Fall 2014, UCI
- American Association of Hispanics in Higher Education respondent for Graduate Fellows, 2014
- Student Mentor for STOVS summer bridge program, Villanova University, 2014
- UCI Molecular Dynamics Seminar Organizer, 2013-2015