

# Stefan Seritan

## EDUCATION

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- 2015 – Present **Graduate Student (Ph.D. Candidate)**  
PHYSICAL CHEMISTRY  
*Stanford University*
- 2011 – 2015 **Bachelor of Science**  
CHEMISTRY AND BIOCHEMISTRY  
*University of California, Santa Barbara*  
GPA: 3.83/4.0

## HONORS & AWARDS

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- 2017 **Linus Pauling Teaching Award**  
*Department of Chemistry, Stanford University*
- 2016 **NSF Graduate Research Fellowship**  
*National Science Foundation*
- 2014 **ACS 248th National Meeting Undergraduate Poster Award**  
*American Chemical Society, COMP Division*
- 2014 **Summer Undergraduate Research Fellowship**  
*University of California, Santa Barbara*
- 2013 **Undergraduate Research and Creative Activities Grant**  
*University of California, Santa Barbara*

## RESEARCH EXPERIENCE

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Graduate Researcher JUL. 2015 - PRESENT  
*Martinez Group*  
*Stanford University*

- Improving real-time interactive molecular dynamics simulations, utilizing the Unity game engine, haptic controllers, and extended reality headsets
- Built a distributed cloud framework for asynchronous GPU-accelerated electronic structure calculations using Docker and Kubernetes
- Benchmarked a rank-reduced full configuration-interaction method
- Investigating reaction networks in shocked HE materials, substituent effects in cyclobutene mechanochemistry, and excitation energy transfer in multichromophoric assemblies
- System administrator for a HPC cluster with over 100 nodes and over 300 GPUs

🏠	380 Roth Way, Rm. 177, Stanford, CA 94305
✉	sseritan@stanford.edu
🌐	<a href="https://www.stefanseritan.com">https://www.stefanseritan.com</a>
in	<a href="https://lnkd.in/stefan-seritan">https://lnkd.in/stefan-seritan</a>
🔄	<a href="https://github.com/sseritan">https://github.com/sseritan</a>
📁	<a href="https://bitbucket.org/sseritan">https://bitbucket.org/sseritan</a>

## RESEARCH EXPERIENCE CONT.

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Undergraduate Researcher MAR. 2013 - JUN. 2015  
*Peters Group*  
*University of California, Santa Barbara*

- Investigated the reactivity of activated methyltriox-orhenium with cyclohexene to form epoxides in solution using DFT
- Implemented a sequential quadratic programming algorithm to study the structure of amorphous supports in catalytic systems
- Studied the effect of a surfactant additive to crystal nucleation in solution using a Potts lattice gas model and Monte Carlo simulations
- Worked on an extended Gibbs ensemble model to study solid-solid phase equilibria

Laboratory Intern JAN. 2010 - JUN. 2010  
*Drs. Florin and Sanda Despa*  
*University of California, Davis*

- Studied the effects of islet amyloid polypeptides (IAPP) and apoptosis on cardiac myocytes, and searched for IAPP in human heart tissue samples. Lab experience includes:
  - Confocal laser microscopy
  - Western blots
  - Gel electrophoresis
  - Fluorescence imaging

## TEACHING EXPERIENCE

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Head Teaching Assistant SEP. 2017 - DEC. 2017  
*Stanford University* OCT. 2016 - DEC. 2016

Teaching Assistant APR. 2016 - JUN. 2016  
*Stanford University* SEP. 2015 - DEC. 2015

Campus Learning Assistance Services Tutor OCT. 2014 - MAR. 2015  
*University of California, Santa Barbara*

Learning Assistant SEP. 2012 - DEC. 2012  
*University of California, Santa Barbara*

## PUBLICATIONS

### Journal Articles

1. Fales, B.S.; **Seritan, S.**; Settje, N.F.; Levine, B.G.; Koch, H.; Martínez, T.J. Large Scale Electron Correlation Calculations: Rank-Reduced Full Configuration Interaction *J. Chem. Theor. Comp.* **2018**, *14* (8), 4139–4150.  
DOI: 10.1021/acs.jctc.8b00382
2. Goldsmith, Z.K.; Provazza, J.; **Seritan, S.** Viewpoints on the 2017 American Conference of Theoretical Chemistry. *J. Phys. Chem. A* **2017**, *121* (41), 7807–7812.  
DOI: 10.1021/acs.jpca.7b09624
3. Goldsmith, B.R.; Hwang, T.; **Seritan, S.**; Peters, B.; Scott, S.L. Rate-Enhancing Roles of Water Molecules in Methyltrioxorhenium-Catalyzed Olefin Epoxidation by Hydrogen Peroxide. *J. Am. Chem. Soc.* **2015**, *137* (30), 9604–9616.  
DOI: 10.1021/jacs.5b03750
4. Seritan, A.L.; **Seritan, S.** Geriatric Psychopharmacology in Acute Settings. *Curr. Psychopharmacol.* **2015**, *4* (2), 112–118.  
DOI: 10.2174/221155600402160201125256
5. Poon, G.; **Seritan, S.**; Peters, B. FD Nucleation: A design equation for low dosage additives that accelerate nucleation *Faraday Discuss.* **2015**, *179*, 329–341.  
DOI: 10.1039/C4FD00226A
6. Seritan, A.L.; Ortigas, M.; **Seritan, S.**; Bourgeois, J.A.; Hagerman, R. Psychiatric disorders associated with FX-TAS. *Curr. Psychiatry Rev.* **2013**, *9*, 59–64.  
DOI: 10.2174/157340013805289699

## PROFESSIONAL ORGANIZATIONS

Student Member <i>American Chemical Society</i>	MAR. 2013 - MAR. 2019
Student Member <i>American Association for the Advancement of Science</i>	APR. 2015 - APR. 2016
Honorary Member <i>Phi Lambda Upsilon, National Chemistry Honor Society</i>	SEP. 2014 - JUN. 2015

## PRESENTATIONS

### Posters

1. **Seritan, S.**; Thompson, K.; Martínez, T.J. A RESTful Framework for Distributed GPU-Accelerated Electronic Structure. West Coast Theoretical Chemistry Symposium, Stanford University, CA, March 2018.
2. **Seritan, S.**; Martínez, T.J. *Ab Initio* Interactive Molecular Dynamics: A Hands-On Experience with Quantum Chemistry. American Conference of Theoretical Chemistry, Boston University, MA, July 2017.
3. **Seritan, S.**; Martínez, T.J. Constructing an Intuitive Virtual Reality Interface for Interactive *Ab Initio* Molecular Dynamics. Theory and Applications of Computational Chemistry Conference, Seattle, WA, & UCLA IPAM DFT Summer School, Los Angeles, CA, August 2016.
4. **Seritan, S.**; Peters, B. Development of an extended Gibbs ensemble for the study of solid-solid phase equilibria. College of Creative Studies Science Week, Santa Barbara, CA, October 2014.
5. **Seritan, S.**; Goldsmith, B.R.; Peters, B. A systematic *ab initio* strategy for predicting structure-activity relationships in amorphous catalysts and supports. ACS 248<sup>th</sup> National Meeting, San Francisco, CA, August 2014.
6. **Seritan, S.**; Goldsmith, B.R.; Peters, B. Computational tools for studies of catalysis on amorphous supports. UCSB Undergraduate Research Colloquium, Santa Barbara, CA, May 2014.
7. **Seritan, S.**; Despa, F.; Despa, S. IAPP and injury of cardiac myocytes. ROP Biotechnology Symposium, Davis, CA, May 2010.

## SKILLS

Programming Languages	Highly Proficient in C, C++, C#, PYTHON Moderately Experienced in CUDA, FORTRAN, JAVASCRIPT, JAVA, RUBY, HTML, CSS
Computer Skills	Bash, Makefiles, Linux Administration (DHCP, DNS, NIS, TFTP), Numerical Libraries (cuBLAS/BLAS, NumPy/SciPy), Microsoft Office Suite, Visual Studio, Unity, Docker, Kubernetes
Languages	Fluent in English Conversational in Romanian