

# Dr. Stefan Seritan

## EDUCATION

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- 2015 – 2020 **Ph.D.**  
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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- 2019 **Falling Walls Lab Finalist**  
*Falling Walls*
- 2019 **OMSC Workshop Travel Grant**  
*Molecular Science Software Institute*
- 2019 **FMA Fellow**  
*SystemX Alliance, Stanford University*
- 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 (2 PFLOPS of compute power)

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🐦	<a href="https://twitter.com/sseritan">https://twitter.com/sseritan</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

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1. Federov, D.; **Seritan, S.**; Fales, B.S.; Martínez, T.J.; Levine, B. PySpawn: Software for Nonadiabatic Quantum Molecular Dynamics. *J. Chem. Theory Comput.* **2020**, *Accepted*.
2. Fales, B.S.; Curtis, E.R.; Johnson, K.G.; Lahana, D.; **Seritan, S.**; Wang, Y.; Weir, H.; Martínez, T.J.; Hohenstein, E.G. Performance of Coupled-Cluster Singles and Doubles on Modern Stream Processing Architectures. *J. Chem. Theory Comput.* **2020**, *Accepted*. DOI: 10.1021/acs.jctc.0c00336
3. **Seritan, S.**; Bannwarth, C.; Fales, B.S.; Hohenstein, E.G.; Kokkila-Schumacher, S.I.L.; Luehr, N.; Snyder, J.; Song, C.; Titov, A.L.; Ufimtsev, I.; Martínez, T.J. TeraChem: Accelerating Electronic Structure and Ab Initio Molecular Dynamics with Graphical Processing Units. *J. Chem. Phys.* **2020**, *152* (22), 224110. DOI: 10.1063/5.0007615
4. **Seritan, S.**; Bannwarth, C.; Fales, B.S.; Hohenstein, E.G.; Isborn, C.; Kokkila-Schumacher, S.I.L.; Li, X.; Liu, F.; Luehr, N.; Snyder, J.; Song, C.; Titov, A.L.; Ufimtsev, I.; Wang, L.-P.; Martínez, T.J. TeraChem: A graphical processing unit-accelerated electronic structure package for large-scale ab initio molecular dynamics. *WIREs Comput. Mol. Sci.* **2020**, *e1494*. DOI: 10.1002/wcms.1494
5. **Seritan, S.**; Thompson, K.; Martínez, T.J. TeraChem Cloud: A High-Performance Computing Service for Scalable Distributed GPU-Accelerated Electronic Structure Calculations. *J. Chem. Inf. Model* **2020**, *60* (4), 2126-2137. DOI: 10.1021/acs.jcim.9b01152
6. 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
7. 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
8. 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
9. Seritan, A.L.; **Seritan, S.** Geriatric Psychopharmacology in Acute Settings. *Curr. Psychopharmacol.* **2015**, *4* (2), 112-118. DOI: 10.2174/221155600402160201125256
10. 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
11. Seritan, A.L.; Ortigas, M.; **Seritan, S.**; Bourgeois, J.A.; Hagerman, R. Psychiatric disorders associated with FXTAS. *Curr. Psychiatry Rev.* **2013**, *9*, 59-64. DOI: 10.2174/157340013805289699

## PRESENTATIONS

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### Talks

1. **Seritan, S.**; Thompson, K.; Martínez, T.J. TeraChem Cloud: A Distributed Framework for GPU-Accelerated Quantum Chemistry. SystemX November Conference, Stanford, CA, USA, November 2019.
2. **Seritan, S.**; Thompson, K.; Martínez, T.J. Breaking the Wall of Quantum Chemistry Accessibility. Falling Walls Lab Finals 2019, Berlin, Germany, November 2019.
3. **Seritan, S.**; Martínez, T.J. Nonadiabatic Dynamics Study of the B800-B850 Complex in LH2 with TeraChem Cloud. OMSC Workshop at EUCO-CTC 2019, Perugia, Italy, September 2019.

### Posters

1. **Seritan, S.**; Johnson, K.G.; Thompson, K.; Hohenstein, E.G.; Martínez, T.J. Frameworks for Distributing a GPU-Accelerated *Ab Initio* Exciton Model. Northern California Theoretical Chemistry Meeting, UC Berkeley, CA, May 2019.
2. **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.
3. **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.
4. **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.
5. **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.
6. **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.
7. **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.
8. **Seritan, S.**; Despa, F.; Despa, S. IAPP and injury of cardiac myocytes. ROP Biotechnology Symposium, Davis, CA, May 2010.

## SKILLS

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Programming Languages	Highly Proficient in C, C++, , PYTHON Experienced in CUDA, FORTRAN, C# 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 Proficient in Romanian