Stefan Seritan

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Education

2015 – 2020 (expected) **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

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 Activitives Grant**
University of California, Santa Barbara

Research Experience

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)

Research Experience Cont.

Undergraduate Researcher
Mar. 2013 - Jun. 2015
Peters Group
University of California, Santa Barbara

- Investigated the reactivity of activated methyltrioxorhenium 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

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: 10.2174/2211556004021602011125256
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: 10.2174/15734001380528969

Professional Organizations

Student Member — Mar. 2013 - Mar. 2019
American Chemical Society

Student Member — Apr. 2015 - Apr. 2016
American Association for the Advancement of Science

Honorary Member — Sep. 2014 - Jun. 2015
Phi Lambda Upsilon, National Chemistry Honor Society

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 Proficient in Romanian

Presentations

Talks

1. **Seritan, S.** 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 248th 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.