Dr. Stefan Seritan

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Objective

Find employment as a research scientist or developer of software infrastructure for scientific research, ideally on applications with broad societal impact and/or increased accessibility of science to the general public.

Relevant Skills:

- Experience with small molecule application projects using density functional theory and configuration-interaction methods
- Participated in development of correlated and fragment-based electronic structure methods
- Proficient in C, C++, C#, Python, CUDA programming languages
- Familiar with build systems on Linux, Mac, and Windows (e.g. Makefiles, CMake, XCode, Visual Studio)
- Fair understanding of Linux system administration (e.g. DHCP, DNS, NIS, IPMI, PXE)
- Deployment on AWS EKS using Docker and Kubernetes containerization technologies
- Familiarity with extended reality through the Unity game engine

Education

2015 – 2020 **Ph.D.** — Stanford University
Physical Chemistry

2011 – 2015 **Bachelor of Science** — University of California, Santa Barbara
Chemistry and Biochemistry

Research Experience

Graduate Researcher — Jul. 2015 - Present
Advisor: Todd Martínez — Stanford University

- Improving real-time interactive molecular dynamics simulations, utilizing the Unity game engine, haptic controllers, and extended reality headsets
  - *Selected Poster:* **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.
- Built a distributed cloud framework for asynchronous GPU-accelerated electronic structure calculations using Docker and Kubernetes, applied to dataset generation and energy transfer in multichromophoric assemblies
  - *Selected Paper:* **Seritan, S.**; Thompson, K.; Martínez, T.J. TeraChem Cloud: A High-Performance Computing Service for Scalable Distributed GPU-Accerelated Electronic Structure Calculations. *J. Chem. Inf. Model*, **2020**, *60 (4)*, 2126-2137. DOI: 10.1021/acs.jcim.9b01152
- Benchmarked a rank-reduced full configuration-interaction method
  - *Selected Paper:* Fales, B.S.; **Seritan, S.**; Settje, N.F.; Levine, B.G.; Koch, H.; Martínez, T.J. *J. Chem. Theor. Comp.* **2018,** *14(8),* 4139-4150. DOI: 10.1021/acs.jctc.8b00382
- Investigating reaction networks in shocked HE materials and substituent effects in mechanochemistry
- System administrator for a Linux HPC cluster with over 100 nodes and over 300 GPUs
- Contributed to a tensor tree linear algebra library designed for quantum dynamics and quantum computing

Undergraduate Researcher — Mar. 2013 - Jun. 2015
Advisor: Baron Peters — University of California, Santa Barbara

- Investigated epoxidation formation of activated methyltrioxorhenium with cyclohexene in solution using DFT
  - *Selected Paper:* Goldsmith, B.R.; Hwang, T.; **Seritan, S.**; Peters, B.; Scott, S.L. *J. Am. Chem. Soc.* **2015,** *137 (30),* 9604-9616. DOI: 10.1021/jacs.5b03750
- Studied the effect of a surfactant additive to crystal nucleation in solution using a Potts lattice gas model and Monte Carlo simulations
  - *Selected Paper:* Poon, G.; **Seritan, S.**; Peters, B. *Faraday Discuss.* **2015,** *179,* 329-341. DOI: 10.1039/C4FD00226A
- Implemented a sequential quadratic programming algorithm to study the structure of amorphous supports in catalytic systems
  - *Selected Poster:* **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. **Conference poster award**
- Worked on an extended Gibbs ensemble model to study solid-solid phase equilibria

Professional 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

Honors & Awards

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 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