Maxwell Venetos

(93 7) 6 8 9 - 7 7 1 8 | mvenetos@berkeley.edu
https://www.linkedin.com/in/maxwell-venetos-a838b3134/

EDUCATION

University of California, Berkeley, Berkeley, CA — Expected: December 2023
PhD of Materials Science and Engineering
Minor in Machine Learning and Quantum Chemistry
NSF Graduate Research Fellow

The Ohio State University, Columbus, OH — December 2019
Bachelor of Science with Research Distinction in Chemistry

PROGRAMMING PROJECTS

GitHub: https://github.com/mVenetos97

mrsimulator

- Co-maintainer of nuclear magnetic resonance simulation code written in Python and C.
- Designed and developed signal processing and data fitting libraries.

nmrcryspy

- Developer and maintainer of NMR crystallography toolkit written in Python.
- Designed fully automated workflows for common NMR crystallography tasks.
- I/O interfaces with common quantum chemical software.

EXPERIENCE

Graduate Student Researcher — **August 2020 – Present**
UC Berkeley, Persson Group — Berkeley, California

- Performs molecular ab initio calculations to model the thermodynamics of polymerization and depolymerization of novel monomers to design recyclable materials.
- Oversees quality control of 29Si NMR calculation database and has grown the database to include additional high quality DFT NMR data.
- Demonstrated that 29Si NMR tensor anisotropy is determined by structure and subsequently built and benchmarked a machine learning model to predict full NMR tensors in silicate materials.
- Designed a workflow to analyze experimental chemical reactions and NMR spectra for novel reaction mixtures and determine the molecules present with no reliance on an external library of spectra.

Research Assistant in Physical Chemistry — **August 2017 – August 2020**
Ohio State University Department of Chemistry, Grandinetti Group — Columbus, Ohio

- Constructed mathematical model using theoretical principals to describe dependence of silicon chemical shift on local geometry. Optimized model for experimental observation using data science techniques.
- Wrote Python scripts for parsing, analysis, and visualization of Gaussian and NMR data.

Teaching Assistant in Organic Chemistry **August 2018 – May 2020**
Ohio State University Department of Chemistry Columbus, Ohio

- Demonstrated Laboratory techniques and Led 20 students in correctly performing laboratory tasks and solving problems weekly.
- Drove efforts to digitize teaching materials to successfully deliver instruction during the Covid-19 pandemic.

Research Assistant in Molecular Engineering **Summer 2018**
Institute of Molecular Engineering at The University of Chicago, Rowan Group Chicago, Illinois

- Synthesized stimuli-responsive polymer films and optimized UV photo-healing conditions for damage in polymer films.
- Analyzed effectiveness of various dyes in photo-healing and adhering polymer sheets.

Student Intern in Responsive Photonic Materials Laboratory **Summer 2016 and Summer 2017**
Wright-Patterson Air Force Base Dayton, Ohio

- Generated and patterned liquid crystal elastomer films to support concentration and stimuli-response study.
- Designed and led research project focusing on development of synthesis methodology for blue-phase liquid crystal films in highly chiral cholesteric samples.

SKILLS

- **Programming Languages** – C++, Python,
- **Machine Learning** – PyTorch, sklearn, JAX, RDKit, Open Babel.
- **Version Control** – Git.
- **Quantum Chemistry** – Gaussian'16, QChem.

PUBLICATIONS

M. C. Venetos, M. Wen, K. Persson, (2023). Machine learning full NMR chemical shift tensors of silicon oxides with equivariant graph neural networks. J. Phys. Chem. A. DOI: https://doi.org/10.1021/acs.jpca.2c07530

M. C. Venetos, S. Dwaraknath, K. A. Persson (2021). Effective Local Geometry Descriptor for 29Si NMR Q4 Anisotropy. The Journal of Physical Chemistry C 125 (35), 19481-19488. DOI: https://doi.org/10.1021/acs.jpcc.1c04829

M. C. Venetos, (2019). Modeling 29Si Chemical Shift in Crystalline and Amorphous Silicas. The Ohio State University Undergraduate Thesis. URL: http://hdl.handle.net/1811/88705

A. R Epstein, E. W. C. Spotte-Smith, **M. C. Venetos**, O. Andriuc, K. A. Persson, (2023). Assessing the Accuracy of Density Functional Approximations for Predicting Hydrolysis Reaction Kinetics. DOI: 10.26434/chemrxiv-2023-c8h70

Brannum, M. T., Steele, A. M., **Venetos, M. C.,** Korley, L. T. J., Wnek, G. E., & White, T. J. (2019). Light Control with Liquid Crystalline Elastomers. Advanced Optical Materials, 1801683. doi:10.1002/adom.201801683

PRESENTIONS

"Mathematical Modeling of ^{29}Si Isotropic Chemical Shifts of Crystalline Silicas" Devon Walter Meek Lecture Poster Session, Ohio State University, Columbus, Ohio, November 2019

"Liquid Crystal Polymer Networks Retaining the Blue Phase Over Wide Temperature Ranges" ACS Dayton Chapter Poster Forum, Dayton, Ohio, April 2018

"Liquid Crystal Polymer Networks Retaining the Blue Phase Over Wide Temperature Ranges" Denman Undergraduate Research Forum, Ohio State University, Columbus, Ohio, April 2018

"Fabrication of Liquid Crystalline Polymer Networks Retaining the Blue Phase" Wright Patterson Air Force Base Summer Intern Research Presentation, Dayton, Ohio, August 2017

"A Concentration Study of Chiral Dopant in Cholesteric Liquid Crystal Cells," Wright Patterson Air Force Base Summer Intern Research Presentation, Dayton, Ohio, August 2016

AWARDS And HONORS

National Science Foundation Graduate Research Fellowship (NSF GRFP) recipient, 2022

Ohio State DataI/O Best Insights from Data Analysis, 2019

Ohio State University Department of Chemistry and Biochemistry Gary Booth Scholarship Recipient, 2018

Most Outstanding Undergraduate Poster, ACS Dayton Chapter Poster Forum, 2018