Pablo Andres Unzueta

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Education

Postdoctoral Research Fellow — July 1, 2022 – Present
Stanford University
Advisor: Professor Todd J. Martínez

Ph.D. in Chemistry — June 2017 – June 2022
University of California, Riverside
Dissertation Advisor: Professor Gregory J. O. Beran

B.S. in Chemistry — September 2012 – June 2017
Cal Poly Pomona

Awards & Fellowships

Mathematical & Physical Sciences Ascending Postdoctoral Fellowship – **$300,000** (National Science Foundation)	2022 – 2025
Advancing Faculty Diversity Fellowship (UC Riverside) – **$35,000**	2021 – 2022
Office of Science Graduate Student Research Award (Department of Energy) – **$18,000**	2021 – 2022
Outstanding Student Poster Award (American Chemical Society Spring Meeting)	2022
Outstanding Teaching Assistant Award (UC Riverside)	2022
Chemistry Alumni Award (UC Riverside) – **$1,000**	2021
Dean's Distinguished Fellowship (UC Riverside) – **$10,000**	2017
Undergraduate Award in Inorganic Chemistry (American Chemical Society)	2017
Research Initiative for Scientific Enhancement Fellowship Program – **$15,000** (Cal Poly Pomona)	2015 – 2017
Minority Health and Health Disparities International Research Training – **$2,000** Fellowship Program (Cal State Fullerton & Universidad Nacional de San Martín)	2016

Interests & Skills

Research Areas	Computational Chemistry, Machine Learning for Quantum Chemistry, Nuclear Magnetic Resonance Chemical Shift Prediction
Systems	Linux and Windows
Programming	Proficient in Python and BASH scripting Familiar with C++, Fortran, and MATLAB
Computational Chemistry	Gaussian, ORCA, QChem, PSI4, Quantum Espresso, CASTEP, Tinker, VMD, Pymol, Mercury
Machine Learning	TensorFlow, PyTorch, PyTorch-Geometric, and Sci-kit Learn
High-Performance Computing	Slurm and PBS computing systems
Languages	English (fluent) and Spanish (advanced)
Professional Memberships	American Chemical Society (March 2020–Present)

Publications

1. **Unzueta, Pablo A.**, Chandler S. Greenwell, and Gregory J. O. Beran. 2021. "Predicting Density Functional Theory-Quality Nuclear Magnetic Resonance Chemical Shifts via Δ-Machine Learning." Journal of Chemical Theory and Computation 17 (2): 826–40.

2. **Unzueta, Pablo A.**, and Gregory J. O. Beran. 2020. "Polarizable Continuum Models Provide an Effective Electrostatic Embedding Model for Fragment-Based Chemical Shift Prediction in Challenging Systems." Journal of Computational Chemistry 41 (26): 2251–65.

3. Dračínský, Martin, **Pablo Unzueta**, and Gregory J. O. Beran. 2019. "Improving the Accuracy of Solid-State Nuclear Magnetic Resonance Chemical Shift Prediction with a Simple Molecular Correction." Physical Chemistry Chemical Physics: 21 (27): 14992–0.

Projects

Density Functional Theory-Based Nuclear Magnetic Resonance Chemical Shift Prediction June 2017 – June 2022
Advisor: Greg Beran

- Development of fragment-based NMR shift prediction methods into in-house Hybrid Many-Body Interaction (HMBI) code.
- Neural networks for NMR chemical shift prediction.
- High-performance computing for chemical shift prediction in proteins, molecular crystals, and machine learning dataset creation.

Improving Graph Convolution Neural Network Architectures for Property Prediction September 2021 – May 2022
Advisor: Victor Fung (Oak Ridge National Lab)

- Office of Science Graduate Student Research Award (Department of Energy)
- GPU-based implementation of graph convolution neural networks for improving property predictions (e.g. NMR chemical shifts) using pytorch in MatDeepLearn.
- Active learning data-scheme with improved graph convolution operators for "universal" quantum chemistry feature descriptors.

Investigating (3-oxo-3-phenyl-1-propen-yl)-Ferrocene and its derivatives as antimicrobial agents April 2015 – May 2017
Advisor: Francis Flores (Cal Poly Pomona)

- Synthesis and NMR characterization of ferrocenyl–chalcone compounds for mechanistic discovery.
- Specialized in stopped-flow UV–Vis spectroscopy.
- Lead lab organizer for chemical ordering, training, and waste disposal.

Effector protein screening of *Brucella abortus* using bacterial adenylate cyclase two hybrid (BACTH) system June 2016 – August 2016
Advisor: Diego Comerci (Universidad Nacional de San Martín, Buenos Aires, Argentina)

- 10-week microbiology training program in Argentina for identifying key proteins involved in host interactions for *B. abortus*.
- Techniques used: flame sterilization, medium growth, plating, recombinant DNA vector introduction, DNA purification, laminar flow.

Talks

ACS Spring 2021 Meeting (Virtual) April 9, 2021
"Improving the accuracy and efficiency of nuclear magnetic resonance chemical shift predictions for molecular crystals"

Cal Poly Pomona Chemistry Seminar (Virtual) March 4, 2021
"Combining Data Science and Chemistry: Highly Accurate Nuclear Magnetic Resonance Chemical Shift Predictions via Δ-Machine Learning"

(Canceled: COVID-19) ACS Spring 2020, Philadelphia, PA March 2020
"Low-cost strategies for predicting chemical shifts more accurately"

Cal Poly Pomona Biological Sciences Seminar, Pomona, CA October 2018
"Fragment–Based Nuclear Magnetic Resonance Chemical Shift Predictions in Proteins and Molecular Crystals"

Posters

ACS Spring 2022 Meeting (San Diego) March 23, 2022
"Machine learning methods for reproducing density functional theory-based nuclear magnetic resonance chemical shifts"

Service

Vice President of Internal Fairs September 2019 – June 2020
Graduate Student Association (UC Riverside)

- Coordinated graduate student efforts for diversity and inclusion, food and housing insecurity, professional development, and campus sustainable practices.
- Routinely met with liaisons from various campus entities and campus leadership, sat on the Research and Scholarly Distinction Board, Highlander Union Building Governing Board, and Student Recreation Governing Board.
- Worked closely with graduate student association elected board, co-chaired monthly meetings, and aided graduate students to transition online during initial stages of COVID–19.

Teaching

Teaching Assistant (UC Riverside Chemistry)

- CHEM 113: Quantum Mechanics Discussion — Spring 2021
- CHEM 111L: Physical Chemistry Lab — Winter 2019
- CHEM 001LC: General Chemistry Lab C — Spring 2020
- CHEM 001LB: General Chemistry Lab B — Winter 2018
- CHEM 001LA: General Chemistry Lab A — Fall 2017, Fall 2019