Jesús Valdiviezo

Computational Chemist · Machine Learning Engineer · Fulbright Alumnus

Duke University — Department of Chemistry, and Department of Electrical and Computer Engineering
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Education

Ph.D. in Computational Chemistry — *Durham, U.S.*

Duke University — *Aug. 2016 – Exp. Jul. 2021*

- Certificate in Nanoscience and Certificate in College Teaching.
- Dissertation: Theory and Simulations of Charge Transport in Engineered Chemical Systems.
- Advisor: Prof. David N. Beratan.

M.S. in Electrical and Computer Engineering — *Durham, U.S.*

Duke University — *Aug. 2019 – Exp. Jul. 2021*

- Concentration in Data Analytics and Machine Learning.

B.S. in Chemistry — *Monterrey, Mexico*

Tecnologico de Monterrey — *Aug. 2011 – May 2016*

- Graduated with honors and the highest chemistry grade point average.
- Research and Innovation Modality and Diploma in Student Development.
- Studied abroad in Germany at Karlsruhe Institute of Technology.
- Thesis: Molecular Rectification Enhancement Based on Conformational and Chemical Modifications: Smart Design of Molecular Devices.
- Advisors: Prof. Julio L. Palma and Prof. Marcelo Videa.

Professional Experience

Co-Founder — *Durham, U.S.*

E-Sentience LLC — *Dec. 2019 – Present*

- Building a startup on AI-powered microfluidic devices.

Research and Teaching Assistant — *Durham, U.S.*

Duke University — *Aug. 2016 – Present*

- Conducting research on nanoscale materials.
- Taught graduate-level Physical Chemistry courses.

Research Assistant — *Tempe, U.S.*

The Biodesign Institute at Arizona State University — *Jun. 2013 – Aug. 2013*

- Conducted research on bioinspired molecular electronics.

Teaching Experience

Quantum Dynamics | CHEM 590 (Graduate-level Course) — *Durham, U.S.*

Duke University — *Fall 2020*

- Curriculum design and instruction. 15 Students.
- Wrote textbook chapters and Python scripts for Quantum Dynamics simulations.

Molecular Simulation | CHEM 590 (Graduate-level Course) — *Durham, U.S.*

Duke University — *Spring 2020*

- Curriculum design and instruction. 15 students.

Skills

Language Skills

English	Fluent (TOEFL iBT: 104, 2015).
Spanish	Native speaker.
German	Good command (Goethe-Zertifikat B1, 2014).
Korean	Basic communication skills.

Computer Skills

Languages	Bash, C/C++, Python (NumPy, SciPy, Pandas, Matplotlib, Scikit-learn, Pytorch), MATLAB, Mathematica, HTML&CSS, LaTeX.
Software	Gaussian, Orca, GAMESS (US), Dalton, Turbomole, Q-Chem, TranSIESTA, Rosetta, NAMD, VMD, Autodock, ChemDraw.

Publications

Peer–Reviewed Journal Articles

1. J. Valdiviezo, P. Zhang and D. N. Beratan. Electron Ratcheting in Self-Assembled Soft Matter. *J. Chem. Phys.*, **In Review**.
2. J. Valdiviezo†, C. Clever†, E. Beall, A. Pearse, Y. Bae, P. Zhang, C. Achim, D. N. Beratan and D. H. Waldeck. Delocalization-Assisted Transport through Nucleic Acids in Molecular Junctions. *Biochemistry*, **2021**, 60(17), pp.1368-1378.
3. J. Valdiviezo†, P. Rocha†, A. Polakovsky and J. L. Palma. Nonexponential Length Dependence of Molecular Conductance in Acene-Based Molecular Wires. *ACS Sens.*, **2021**, 6(2), pp.477-484.
4. A. Polakovsky, J. Showman, J. Valdiviezo and J. L. Palma. Quantum Interference Enhances Rectification Behavior of Molecular Devices. *Phys. Chem. Chem. Phys.*, **2021**, 23(2), pp.1550-1557.
5. X. Li†, J. Valdiviezo†, S. D. Banziger, P. Zhang, T. Ren, D. N. Beratan and I. V. Rubtsov. Symmetry Controlled Photo-Selection and Charge Separation in Butadiyne-Bridged Donor–Bridge–Acceptor Compounds. *Phys. Chem. Chem. Phys.*, **2020**, 22(17), pp.9664-9676.
6. S. D. Banziger†, X. Li†, J. Valdiviezo, M. Zeller, P. Zhang, D. N. Beratan, I. V. Rubtsov and T. Ren. Unsymmetrical Bis–Alkynyl Complexes Based on Co(III)(cyclam): Synthesis, Ultrafast Charge Separation and Analysis. *Inorg. Chem.*, **2019**, 58(22), pp.15487-15497.
7. J. Valdiviezo and J. L. Palma. Molecular Rectification Enhancement Based on Conformational and Chemical Modifications. *J. Phys. Chem. C.*, **2018**, 122(4), pp.2053–2063.

Books

1. D. N. Beratan., J. Valdiviezo, J. Yuly and P. Zhang. Dynamical Chemistry: A Hands-on Guidebook for Understanding Coherence Phenomena in Chemistry. **In Preparation**.

† Contributed equally.

Selected Honors and Awards

Rice Academy Postdoctoral Fellowship, Rice University (Declined) — ***Houston, U.S.*** *2021*
FIP Special Student Seminar Award, Fitzpatrick Institute for Photonics at Duke University — ***Durham, U.S.*** *2020*
Kathleen Zielik Fellowship, Duke University Department of Chemistry — ***Durham, U.S.*** *2020*
Bass Graduate School Fellowship, Duke University Graduate School — ***Durham, U.S.*** *2019*
Duke Incubation Fund, The Duke Innovation & Entrepreneurship Initiative — ***Durham, U.S.*** *2019*
Telluride School on Theoretical Chemistry Award, Telluride Science Research Center — ***Telluride, U.S.*** *2019*
Quantum Science Summer School Award, NSF/DOE — ***St College, U.S.*** *2019*
Duke Support for Interdisciplinary Graduate Networks Grant, Duke Interdisciplinary Studies — ***Durham, U.S.*** *2019*
Graduate Program in Nanoscience Fellowship, GPNANO at Duke University — ***Durham, U.S.*** *2018*
Sci-Mix Presentation, ACS Division of Computers in Chemistry — ***Washington, U.S.*** *2017*
CONACYT-Nuevo Leon Fellowship, CONACYT (Declined) — ***Monterrey, Mexico*** *2016*
Excellence Performance Award, CENEVAL — ***GDL, Mexico*** *2015*
Fulbright Scholarship, The Fulbright Program — ***CDMX, Mexico*** *2015*
Xorge A. Dominguez Scholarship, Tecnologico de Monterrey Department of Chemistry — ***Monterrey, Mexico*** *2011*
Academic Talent Scholarship, Tecnologico de Monterrey — ***Monterrey, Mexico*** *2011*

Synergistic Activities

The Triangle Molecular Simulation Society Co-Director — *Durham, U.S.*

The Triangle Molecular Simulation Society — *Aug. 2019 – Present*

- Launched an initiative designed to involve students, researchers, and enthusiasts of molecular simulation.

COMEXUS Selection Process Panelist – Chemistry — *CDMX, Mexico*

COMEXUS Fulbright-Garcia Robles — *May 2021*

- Invited to interview and evaluate Mexican chemistry candidates for the Fulbright Scholarship.

Douglas G. Hill Memorial Lecture Co-Chair — *Durham, U.S.*

Duke Graduate Chemistry Council and the Duke University Department of Chemistry — *Jan. 2019 – Mar. 2021*

- Organizer of The Hill Lecture, the department's most significant external honors.
- Lecturers: Prof. Joanna Aizenberg (Harvard University) and Prof. Stuart Schreiber (Harvard University).

Science Instructor and Mentor — *Latin America*

Science Clubs International — *Apr. 2017 – Mar. 2021*

- Designed and instructed four one-week workshops for high school and college students from Latin America.
- Developed a mini-MOOC (Massive Open Online Course) in solar technologies. Website: minimoocs.clubesdeciencia.mx/