Arturo Sauza de la Vega, Ph.D.

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Personal information

Citizenship: Dual US/Mexican.

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Occupation: Posdoctoral Scholar, Univesity of Iowa.

Education

B.Eng. in Chemical Engineering

- **Institution:** National Polytechnic Institute (IPN), Mexico.
- **Degree granted:** December 2016.

B.Sc. in Chemistry

- **Institution:** National Autonomous University of Mexico (UNAM), Mexico.
- **Degree granted:** January 2018.

M.Sc. in Chemistry

- **Institution:** National Autonomous University of Mexico (UNAM), Mexico.
- **Degree granted:** October 2020.

M.Sc. in Chemistry

- **Institution:** The University of Chicago (UChicago), USA.
- **Degree granted:** November 2021.

Ph.D. in Chemistry

- **Institution:** The University of Chicago (UChicago), USA.
- **Degree granted:** June 2025.

Postdoctoral Scholar

- **Institution:** The University of Iowa (UIOWA), USA.

Conferences

- **XVI International Symposium "Universities Contributions to Teaching, Research and Technology Development", September 2015, Mexico City, Mexico.**

  Conference: Dehydroalanine derivatives conformational analysis using computational quantum chemistry.
- **Symposium "Frontiers in Computational Chemistry 2016", August 2016, Mexico City, Mexico.**

  Poster: Topology of the electron density and non-covalent interactions analysis of dehydroalanine derivatives relevant in medicinal chemistry.
- **XV Mexican Meeting of Theoretical Physical Chemistry, November 2016, Mérida, México**

  Poster: Topology of the electron density and non-covalent interactions analysis of dehydroalanine derivatives relevant in medicinal chemistry.
- **XVI Mexican Meeting of Theoretical Physical Chemistry, November 2017, Puebla, Mexico**

  Poster: Water clusters as bifunctional catalysts in Organic Chemistry. Ethylene Oxide hydrolysis.
- **XVII Mexican Meeting of Theoretical Physical Chemistry, November 2018, Monterrey, Mexico**

  Poster: Study of the hydrogen bond in water clusters with cations and anions through the IQA energy partition.
- **American Chemical Society 2021 Fall Meeting**

  Poster: Metal aryl complex candidates for molecular qubits.
- **American Chemical Society Spring Meeting, March 2022, San Diego, CA, United States of America**

  Presentation: Zero-Field Splitting of Cr(IV) Molecular Qubits: Theoretical Insights.

Publications

- Vallejo Narváez, W. E.; Jiménez, E. I.; Romero-Montalvo, E.; **Sauza-de la Vega, A.**; Quiroz-García, B.; Hernández-Rodríguez, M.; Rocha-Rinza, T. Acidity and basicity interplay in amide and imide self-association. *Chem. Sci.*, **2018**, 9, 4402–4413. DOI: 10.1039/C8SC01020J.
- **Sauza-de la Vega, A.**; Guevara-Vela, J. M.; Rocha-Rinza, T. Cooperativity and anticooperativity in ion-water interactions. Implications in the aqueous solvation of ions. *ChemPhysChem*, **2021**, 22, 1269–1285. DOI: 10.1002/cphc.202000981.
- **Sauza-de la Vega, A.**; Salazar-Lozas, H.; Vallejo Narváez, W. E.; Hernández-Rodríguez, M.; Rocha-Rinza, T. Water clusters as bifunctional catalysts in organic chemistry. The hydrolysis of oxirane and its methyl derivatives. *Org. Biomol. Chem.*, **2021**, 19, 6776–6780. DOI: 10.1039/D1OB01026C.
- **Sauza-de la Vega, A.**; Duarte, L. J. ; Silva, A. ; Skelton, J. ; Rocha-Rinza, T. ; Popelier, P. L. A., Towards and Atomistic Understanding of Polymorphism in Molecular Solids. *Phys. Chem. Chem. Phys.*, **2022**, 24, 11278–11294. DOI: 10.1039/d2cp00457g.
- Aristizabal-Ferreira, V. A.; Guevara-Vela, J. M.; **Sauza-de la Vega, A.**; Martín Pendás, Á.; Fuentes-Pineda, G., Rocha-Rinza, T., Computation of photovoltaic and stability properties of hybrid organic-inorganic perovskites via convolutional neural networks. *Theor. Chem. Acc.*, **2022**, 141, 19. DOI: 10.1007/s00214-022-02875-9.
- **Sauza-de la Vega, A.**; Pandharkar, R. ; Stroscio, G. D. ; Sarkar, A.; Truhlar, D. G.; Gagliardi, L., Multiconfiguration Pair-Density Functional Theory for Chromium(IV) Molecular Qubits. *JACS Au*, **2022**, 2, 2029–2037. DOI: 10.1021/jacsau.2c00306.
- Guevara-Vela, J. M.; **Sauza-de la Vega, A.**; Gallegos, M. Martín Pendás, Á. ; Rocha-Rinza, T., Wave function analyses of scandium-doped aluminum clusters, Al_nSc ($n = 1 - 24$), and their CO_2 fixiation abilities. *Phys. Chem. Chem. Phys.*, **2023**, 25, 18854–18865. DOI: 10.1039/D3CP01730C.
- Kunstelj, Š.; Darù, A.; **Sauza-de la Vega, A.**; Stroscio, G. D.; Edwards, E.; Gagliardi, L.; Wuttig, A., Competitive Valerate Binding Enables RuO_2-Mediated Butene Electrosynthesis in Water. *J. Am. Chem. Soc.*, **2024**, 146, 20584–20593. DOI: 10.1021/jacs.4c01776.
- Hertler, P..; **Sauza-de la Vega, A.**; Darù, A.; Sarkar, A.; Lewis, R.A.; Gagliardi, L.; Hayton, T.W., A Homoleptic Fe(IV) Ketimide Complex with a Low-Lying Excited

State. *Chem. Sci.*, **2024**, 15, 16559-16566. DOI: 10.1039/D4SC04880F.

- Kirlikovali, K. O.; Gómez-Torres, A.; **Sauza-de la Vega, A.**; Darù, A.; Krzyaniak, M. D.; Wasielewski, M. R.; Gagliardi, L.; Farha, O. K., Electronically Tunable Low-Valent Uranium Metallacarboranes. *Inorg. Chem.*, **2025**, 64, 4749-4760. DOI: 10.1021/acs.inorgchem.4c04431
- **Sauza-de la Vega, A.**; Darù, A.; Nofz, S. Gagliardi, L.; Designing Molecular Qubits: Computational Insights into First-Row and Group 6 Transition Metal Complexes. *Chem. Sci.*, **2025**, 16, 12896-12905, DOI: 10.1039/D5SC02544C.
- **Sauza-de la Vega, A.**; Beltrán-Leiva, M. J.; Gagliardi, L.; Batista, E.R.; Yang, P.; Chemical Bonding and Oxidation State Variability in Lanthanide and Actinide Systems with Non-Innocent Ligands. **2025**, *To be submitted for publication* .
- Gullett, K. L.; Silva, C. L.; **Sauza-de la Vega, A.**; Shaw, T. E.; Pereiro, F. A.; Collins, T. S.; Coughlin, E.J.; Lapsheva, E.; Anderson, N. H.; Gaggioli, C.; Zeller, M.; Mullis, M. S.; Shafer, J. C.; Kozimor, S. A.; Gagliardi, L.; Schelter, E. J. .; Bart, S.; Isolation and Characterization of a Pentakis(imido)uranate (VI) Tetraanion. **2026**, *Submitted for publication* .

Research Internships

The University of Manchester

Supervisor: Prof. Paul L.A. Popelier.

Project: Assisting the Quantum Chemical Topology Group on the REG method to develop this project further.

Period: June 1 to August 31, 2019.

University of Minnesota

Supervisor: Prof. Laura Gagliardi.

Project: Molecular qubits in chromium (IV) aryl complexes.

Period: May 25 to August 31, 2020.

Los Alamos National Laboratory. G.T. Seaborg Institute.

Supervisor: Dr. Ping Yang

Project: Comprehensive Study of Lanthanide and Actinide Complexes with Tropolonate/Semiquinonate Ligands.

Period: June 3 to August 30, 2024.

Professional Skills

Languages

- Spanish (Native).
- English (Fluent).

Technical Skills

- Scientific software: Molcas, Gamess-US, Gaussian 16, Aimall, Promolden, Gnuplot, Avogadro, MacMolPlt, Vesta, VMD, IQmol, Orca, ADF, PySCF, Turbomole.
- Editing software: LaTeX, Tikz, Gimp, Inkscape.
- Programming: Bash, Python.
- Operating Systems: Linux, Windows.

Work References

- Prof. Tomás Rocha-Rinza, trocha@iquimica.unam.mx, Institute of Chemistry - UNAM, Mexico.
- Dr. Ping Yang, pyang@lanl.gov, Los Alamos National Laboratory, USA.
- Prof. Laura Gagliardi, lgagliardi@uchicago.edu, The University of Chicago, USA.
- Prof. Bess Vlaisavljevich, bess-vlaisavljevich@uiowa.edu, University of Iowa, USA.
- Dr. María Joaquina Beltrán Leiva, mariab@lanl.gov, Los Alamos National Laboratory, USA.
- Dr. José Manuel Guevara-Vela, j.guevara-vela@hw.ac.uk, Heriot-Watt University, UK.