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Education

Licenciado in Physics	1991-1996	FAMAF. Universidad Nacional de Córdoba, Argentina Advisor: Prof. Horacio M. Pastawsky
Ph.D. in Physical Chemistry	1998-2002	Louisiana State University Advisor: Prof. Randall W. Hall

Academic and Professional Appointments

2018-present	Professor of Chemistry, University of Connecticut, Storrs, CT
2012-2018	Associate Professor of Chemistry, University of Connecticut, Storrs, CT
2006-2012	Assistant Professor of Chemistry, University of Connecticut, Storrs, CT
2002-2006	Postdoctoral Associate, Yale University, New Haven, CT Advisor: Prof. Victor S. Batista
1998-2002	Graduate Teaching Assistant, Louisiana State University, Baton Rouge, LA

Awards

Hewlett Packard Outstanding Junior Faculty Award (2009)
Camille and Henry Dreyfus New Faculty Award (2006)
Career Award, National Science Foundation (2009)
Rudolph J. Anderson Fellowship. Yale University (2002-2003)
Award for Superior Performance and Productivity in Chemical Research, LSU (2000)
Award *Universidad* for special distinction as undergraduate student, UNC (1996)

Publications in Refereed Journals

79 Daniels, R.; Yassin, O. A.; Toribio, J. M.; Gascón, J. A.; Sotzing, G. Re-examining Cannabidiol: Conversion to Tetrahydrocannabinol Using Only Heat. *Cannabis and Cannabinoid Research*. **2022**, ASAP.

78 Nisansala, H.; Guberman-Pfeffer, M. J.; Chaudhri, N.; Zeller, M.; Gascón, J. A.; Brückner, C. Syntheses and Aromaticity Parameters of Hexahydroxypyrrocorphin, Porphotrilactones, and Their Oxidation State Intermediates. *J. Org. Chem.* **2022**, *87*, 12096-12108.

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- 73** Gelpí-Domínguez, S.; Rossi, A. R.; Gascón, J. A. Insights into Diastereotopic Effects in Thiolated Gold Nanoclusters. *Chem. Phys. Lett.* **2021**, *770*, 138448
- 72** Clark, K.; Pigni, N. B.; Wijesiri, K.; Gascón, J. A. Spectral Features of Canthaxanthin in HCP2. A QM/MM Approach. *Molecules* **2021**, *26*, 2441.
- 71** Tilluck, R. W.; Ghosh, S.; Guberman-Pfeffer, M. J.; Roscioli, J. D.; Gurchiek, J. K.; LaFountain, A. M.; Frank, H. A.; Gascón, J. A.; Beck, W. F. Interexciton nonradiative relaxation pathways in the peridinin-chlorophyll protein. *Cell Rep. Phys. Sci.* **2021**, *2*, 100380.
- 70** An, J.; Intano, J.; Richard, A.; Kim, T.; Gascón, J. A.; Howell, A. R. Easily accessible non-aromatic heterocycles with handles: 4-bromo-2, 3-dihydrofurans from 1, 2-dibromohomoallylic alcohols. *Chem. Sci.* **2021**, *12*, 10347-10353
- 69** Saavedra-Avila, N. A.; Keshipeddy, S.; Guberman-Pfeffer, M. J.; Pérez-Gallegos, A.; Saini, N. K.; Schäfer, C.; Carreño, L. J.; Gascón, J. A.; Porcelli, S. A.; Howell, A. R. Amide-Linked C4"-Saccharide Modification of KRN7000 Provides Potent Stimulation of Human Invariant NKT Cells and Anti-Tumor Immunity in a Humanized Mouse Model. *ACS Biology* **2020**, *15*, 3176-3186
- 68** Pigni, N. B.; Clark, K. L.; Beck, W. F.; Gascón, J. A. Spectral Signatures of Canthaxanthin Translocation in the Orange Carotenoid Protein. *J. Phys. Chem. B.* **2020**, *124*, 11387-11395.
- 67** Gurchiek, J. K.; Rose, J. B.; Guberman-Pfeffer, M. J.; Tilluck, R. W.; Ghosh, S.; Gascón, J. A.; Beck, W. F. Fluorescence Anisotropy Detection of Barrier Crossing and Ultrafast Conformational Dynamics in the S₂ State of β-Carotene. *J. Phys. Chem. B.* **2020**, *124*, 9029-9046
- 66** Jolin, W. C.; Richard, A.; Vasudevan, D.; Gascón, J. A.; MacKay, A. A. Aluminosilicate Mineralogy and the Sorption of Organic Cations: Interplay between Electrostatic Barriers and Compound Structural Features. *Environ. Sci. Technol.* **2020**, *54*, 1623-1633.
- 65** Richard, M. A.; Gascón, J. A. Protein polarization effects in the thermodynamic computation of vibrational Stark shifts. *Theor. Chem. Acc.* **2020**, *139*, 1-9.
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- 62** Guberman-Pfeffer, M. J.; Gascón, J. A. Carotenoid-Chlorophyll Interactions in a Photosynthetic Antenna Protein: A Supramolecular QM/MM Approach. *Molecules* **2018**, *23*, 2589-2600
- 61** Yang, B.; Hewage, N.; Guberman-Pfeffer, M. J.; Wax, T.; Gascón, J. A.; Zhao, J.; Agrios, A. G.; Brückner, C. The limited extend of the electronic modulation of chlorins and bacteriochlorins through chromene-annulation. *Phys. Chem. Chem. Phys.* **2018**, *20*, 18233-18240
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- 59** Chennamadhavuni, D.; Saavedra-Avila, N. A.; Carreño, L. J.; Guberman-Pfeffer, M. J.; Arora, P.; Yongqing, T.; Koay, H.; Godfrey, D.; Keshipeddy, S.; Richardson, S. K.; Sundararaj, S.; Lo, J. H.; Wen, X.; Gascón, J. A.; Yuan, W.; Rossjohn, J.; Le Nours, J.; Porcelli, S. A.; Amy R Howell.: Dual Modifications of α -Galactosylceramide Synergize to Promote Activation of Human Invariant Natural Killer T Cells and Stimulate Anti-tumor Immunity. *Cell Chem. Biol.* **2018**, *25*, 1-14.
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- 46** Pahalagedara, M. N.; Samaraweera, M.; Dharmarathna, S.; Kuo, C.-H.; Pahalagedara, L. R.; Gascón, J. A.; Suib, S. L.: Removal of azo dyes: intercalation into sonochemically synthesized NiAl layered double hydroxide. *J. Phys. Chem. C* **2014**, *118*, 17801-17809.
- 45** Ho, J.; Newcomer, M. B.; Ragain, C. M.; Gascón, J. A.; Batista, E. R.; Loria, J. P.; Batista, V. S.: MoD-QM/MM Structural Refinement Method: Characterization of Hydrogen Bonding in the Oxytricha Nova G-quadruplex. *J. Chem. Theor. Comput.* **2014**, *10*, 5125-5135.
- 44** Dainese, T.; Antonello, S.; Gascón, J. A.; Pan, F.; Perera, N. V.; Ruzzi, M.; Venzo, A.; Zoleo, A.; Rissanen, K.; Maran, F.: Au₂₅(SEt)₁₈, a Nearly Naked Thiolate-Protected Au₂₅ Cluster: Structural Analysis by Single Crystal X-Ray Crystallography and Electron Nuclear Double Resonance. *ACS Nano* **2014**, *8*, 3904-3912.
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- 36** Banerjee, S.; Montgomery, J. A.; Gascón, J. A.: A QM/MM Approach for the Study of Monolayer-Protected Gold Clusters. *J. Mater. Sci.* **2012**, *47*, 7686-7692.
- 35** Venzo, A.; Antonello, S.; Gascón, J. A.; Guryanov, I.; Leapman, R. D.; Perera, N. V.; Sousa, A.; Zamuner, M.; Zanella, A.; Maran, F.: Effect of the Charge State ($z = -1, 0, + 1$) on the Nuclear Magnetic Resonance of Monodisperse Au₂₅[S(CH₂)₂Ph]₁₈^z clusters. *Anal. Chem.* **2011**, *83*, 6355-6362.
- 34** Menikarachi, L. C.; Gascón, J. A.: An Extrapolation Method for Computing Protein Solvation Energies Based on Density Fragmentation of a Graphical Surface Tessellation. *J. Mol. Graph. Model.* **2011**, *30*, 38-45.
- 33** Duff Jr, M. R.; Fyvie, W. S.; Markad, S. D.; Frankel, A. E.; Kumar, C. V.; Gascón, J. A.; Peczu, M. W.: Computational and Experimental Investigations of Mono-Septanoside Binding by Concanavalin A: Correlation of Ligand Stereochemistry to Enthalpies of Binding. *Org. Biomol. Chem.* **2011**, *9*, 154-164.

- 32** Beshir, A. B.; Argueta, C. E.; Menikarachchi, L. C.; Gascón, J. A.; Fenteany, G.: Locostatin Disrupts Association of Raf Kinase Inhibitor Protein with Binding Proteins by Modifying a Conserved Histidine Residue in the Ligand-Binding Pocket. *Forum on immunopathological diseases and therapeutics*; Begel House Inc., 2011; Vol. 2.
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- 29** Menikarachchi, L. C.; Gascón, J. A.: QM/MM Approaches in Medicinal Chemistry Research. *Curr. Top. Med. Chem.* **2010**, *10*, 46-54.
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- 24** Menikarachchi, L. C.; Gascón, J. A.: Optimization of Cutting Schemes for the Evaluation of Molecular Electrostatic Potentials in Proteins via Moving-Domain QM/MM. *J. Mol. Model.* **2008**, *14*, 1-9.
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- 5** Gascón, J. A.; Hall, R. W.; Ludewigt, C.; Haberland, H.: Structure of Xe_N⁺ Clusters (N= 3–30): Simulation and Experiment. *J. Chem. Phys.* **2002**, *117*, 8391-8403.
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2 Pastawski, H. M.; Gascón, J. A.: NMR Line Shape in Metallic Nanoparticles: A Matrix Continued Fractions Evaluation. *Phys. Rev. B* **1997**, *56*, 4887- 4902.

1 Pastawski, H.; Gascón, J.; Medina, E.: NMR Characterization of Metallic Nanoparticles: A Manifestation of Mesoscopic Phenomena. In *Anal. Asoc. Quím. Arg.* **1996**, *84*, 397-401.

External Grants

1 NSF. Collaborative Research: Combining Theory and Experiment to Understand the First Photophysical Events in the Photoactivation of the Orange Carotenoid Protein (PI: José Gascón, co-PI: Warren Beck) 9/2022-8/2025 (**\$277,074**).

2 NSF. Harnessing NKT Cell Activation by Glycolipids. (PI: Amy Howell, Co-PIs: José Gascón, Steven Porcelli) (PI: Amy Howell, Co-PIs: José Gascón, Steven Porcelli) 09/2019 – 08/2023 (**\$2,097,577**).

3 Collaborative Research: Combining Theory and Experiment to Understand Carotenoid Photophysics in Photosynthetic Light-Harvesting (PI: José Gascón, co-PI: Warren Beck) 9/2019-8/2022 (**\$327,496**).

4 NIH. Harnessing NKT Cell Activation by Glycolipids. (PI: Amy Howell, Co-PIs: José Gascón, Steven Porcelli) 09/2014 – 08/2018 (**\$2,520,787**).

5 NSF. REU Site: Research Experience for Undergraduates in Chemistry at the University of Connecticut. (PI: José Gascón, co-PI: Alfredo Angeles-Boza). 9/2018-8/2022 (**\$297,000**).

6 NSF-XSEDE. Investigation of the Tuning Mechanism by Means of Protein Environment and Excitonic Coupling in the PCP Complex. (PI: José Gascón). Competitive grant for supercomputing time. (**100,000 SUs**).

7 NSF-ECS. Collaborative Research: Organic Cation Interactions with Soil Aluminosilicates: Structure-Sorption relationships. (PI: José Gascón, co-PI: Allison MacKay) 10/2014-9/2018 (**\$410,000**).

8 NIH. Harnessing NKT Cell Activation by Glycolipids. (PI: Amy Howell, Co-PIs: José Gascón, Steven Porcelli, Weiming Yuan) 09/2014 – 08/2018 (**\$1,946,721**).

9 NSF. REU Site: Research Experience for Undergraduates in Chemistry at the University of Connecticut. PI: Mark Peczu, Co-PI José Gascón. 6/2014-5/2017 (**\$277,526**).

10 NSF Career Award. Scalable Moving-Domain QM/MM Methods for the Computation of Protein Electrostatics. (PI: José Gascón) 9/1/2009-8/30/2014 (**\$600,000**).

11 Camille & Henry Dreyfus Foundation. First Principles determination of structure and activity in biomacromolecules. (PI: José Gascón) 8/23/2006-8/23/2011 (**\$50,000**).

Internal Grants

1 Office of the Vice President for Research. Connectivity-based Force Fields to Model Thiolated Gold Molecular Clusters. (PI: José Gascón) 7/1/2016-6/30/2017 (**\$24,954**).

2 UConn Research Foundation. Towards a First Principles Description of Monolayer-Protected Gold Clusters. (PI: José Gascón) 1/1/2011-31/12/2011 (**\$23,300**).

3 UConn Research Foundation. Quantum Mechanical Refinement of Structure and Electrostatic Properties of Proteins. (PI: José Gascón) 8/1/2007-8/1/2008 (**\$19,000**).

Invited and Contributed Presentations (* = invited)

- 1* QM/MM simulations enable structure spectral relationships in photosynthetic proteins. ACS San Diego. March 21st, **2022**.
- 2* Structure-Spectrum Relationships in a Light Harvesting Antenna: A Supramolecular QM/MM approach. Universidad de Puerto Rico, Rio Piedras, January 16th **2019**.
- 3* Structure-Spectrum Relationships in a Light Harvesting Antenna: A Supramolecular QM/MM approach, Wesleyan University, Middletown, CT. November 16th **2018**.
- 4* Spectral and Structural Relationships in Gold Nanoclusters. Mechanical and Quantum Models. University of Colorado, Denver, CO. February 23rd, **2018**.
- 5* *Biocompatible Force Field for Thiolated Gold Nanoclusters in Macromolecular Environments*. Department of Chemistry. Brown University, RI. November 2, **2017**.
- 6 *Biocompatible Force Field for Thiolated Gold Nanoclusters in Macromolecular Environments*. American Chemical Society National Meeting. San Francisco, CA. April 5th, **2017**.
- 7* *Biocompatible Force Field for Thiolated Gold Nanoclusters in Macromolecular Environments*. El Colegio Nacional. Mexico City, Mexico. March 17th, **2017**.
- 8* *QM/MM Prediction of Electric Fields in the Active site of Proteins: Aiding the Analysis of Stark Shift Measurements*. Department of Chemistry, University of New Haven, CT. January 25th, **2016**.
- 9* *QM/MM Prediction of Electric Fields in the Active site of Proteins: Aiding the Analysis of Stark Shift Measurements*. Department of Chemistry, University of Padova, Italy. May 8th, **2014**.
- 10 *QM/MM Prediction of Electric Fields in the Active site of Proteins: Aiding the Analysis of Stark Shift Measurements*. American Chemical Society National Meeting. Indianapolis, IN. September **2013**.
- 11 *Scalable Quantum Chemical Approaches for the Study of Protected Gold Clusters*. Gordon Research Conference (poster). Holyoke, MA, June 18 **2012**.
- 12* *Moving Domain QM/MM Methods for the Treatment of Polarization Effects in Proteins*. Department of Chemistry. Emory University. Atlanta, GA. September 17th **2011**.
- 13* *Quantum Chemical Detail of Structural Changes and Spectral Tuning in the First Vision Event of Squid Rhodopsin*. School of Chemistry & Biochemistry. Georgia Tech. Atlanta, GA. September 18th **2011**.
- 14* *Quantum Chemical Detail of Structural Changes and Spectral Tuning in the First Vision Event of Squid Rhodopsin*. Department of Chemistry. Georgia State University. Atlanta, GA. September 2nd **2011**.
- 15* *Molecular Simulations of Protein-Ligand Binding*. UConn Early College Experience Workshop. Storrs, CT. May 12th **2011**.
- 16 *Moving domain methods for treatment of polarization effects in proteins*. XVII Argentinean Congress of Physical and Inorganic Chemistry. May 3rd **2011**, Cordoba, Argentina.
- 17* *Quantum Chemical Detail of Structural Changes and Spectral Tuning in the First Vision Event of Squid Rhodopsin*. 1st Argentinean Workshop of Biophysical Chemistry of Proteins. Cordoba, Argentina. May 2nd **2011**.

- 18* *Atomistic Simulations of Proteins and Enzymes*. ISIS (Institute for Science Instruction and Study), UConn. July 7th **2010**.
- 19* *Local and global refinement of protein electrostatics using a Moving-Domain QM/MM approach*. American Physical Society National Meeting. Denver, CO. March **2007**.
- 20* *Quantum Mechanics of Protein Active Sites*. Seminar at Connecticut College. New London, CT. December **2007**.
- 21* *Moving Domain QM/MM method to model the electrostatic potential in bio-macromolecules*. 50th Anniversary of FAMAFA, Universidad Nacional de Cordoba, Argentina. December **2006**.
- 22* *Moving Domain QM/MM method to model the electrostatic potential in bio-macromolecules*. Conn. Valley Quantum Chemistry group. Storrs, CT. December **2006**.

Educational Outreach and Initiatives

- Summer **2019-2022**. Coordinator of the NSF-REU program in the Chemistry Department.
- Summer **2008-2016**. Organized the high school summer program SECRET (*School for Exploratory Chemical Research and Training*). Designed a website for the promotion of SECRET. <http://chemistry.uconn.edu/secret.htm>
- Lead the effort for the University-wide acquisition of the Molecular Modeling Software Schrodinger with a 6-year license agreement (**2016-2022**).
- Summer **2014-2017**. Co-Coordinator of the NSF-REU program the Chemistry Department.
- Academic Year **2015**. Advanced Research Mentorship. Mentored High School from Glastonbury High School on a computational research project.
- Summer 2015. Participated in the ACS-SEED program. Designed and supervised a high school minority student who carried out research on Computational Chemistry.
- Summer **2007, 2009-10**. Participated in the UConn Mentor Connection for the gifted and talented. Designed and supervised high school students who carried out research on Computational Chemistry.
- Spring **2010**. Organized a mini workshop to teach middle school teachers at Windham middle school how to use a molecular modeling software, which I acquired from NSF funds, originally allocated for this purpose as part of the educational component of the CAREER Award.
- University of Connecticut, summer **2007**. Co-founded along with the Junior faculty in the Chemistry Department the outreach program SECRET.

Supervising Activities

- Raian Mahjoob (Ph.D), 2022-present
- Natalia Pigni (postdoc), 2019-2022
- Kithmini Wijesiri (Ph.D), 2019-present
- Kevin Clark (M.S), 2019-2022
- Mansi Malhotra (Ph.D), 2016-present, co-advisor with Prof. Challa Kumar
- Alissa Richard (Ph.D), 2015-2020
- Svetlana Gelpi (Ph.D), 2015-2021
- Matthew Guberman-Pfeffer (Ph.D), 2014-2019
- Jennifer Pardus (M.S), 2008-2016

- George Omolloh (Ph.D), 2011-2013
- Milinda Samaraweera (Ph.D), 2010-2016
- Neranjan Perera (Ph.D), 2008-2015
- Daniel Sandberg (Ph. D), 2010-2012
- Lochana Menikarachchi (Ph.D), 2006-2011
- Alexandra Rudnitskaya (postdoc), 2010-2012
- Yuang Zhang (postdoc), 2006-2008