

Pablo E. Videla, Ph.D.

CONTACT INFORMATION	Department of Chemistry, Yale University 225 Prospect Street, New Haven, CT	(203) 415-9258 pablo.videla@yale.edu
RESEARCH INTERESTS	Structure and dynamics of complex condensed phase systems. Quantum dynamics and nonadiabatic dynamics simulations. Nuclear quantum effects in gas and condensed phases. Statistical mechanics of liquids. Multidimensional spectroscopy.	
EDUCATION	University of Buenos Aires, Argentina	
	<ul style="list-style-type: none">• Ph.D., Physical Chemistry 2015 Advisor: Professor Daniel Laría Thesis: <i>Nuclear Quantum Effects in Aqueous Environments</i>• <i>Licenciado en Ciencias Químicas</i> 2011 (equivalent to M.S., Chemistry)	
RESEARCH EXPERIENCE	Yale University, New Haven, CT	
	<ul style="list-style-type: none">• Postdoctoral Associate in Chemistry 2016-present Advisor: Professor Victor S. Batista Research: Development of computational methods to study how the underlying substrate-adsorbate interactions modulated the orientation, energetics and reactivity of different molecules at interfaces, with particular emphasis on the simulation of surface-specific nonlinear spectroscopies such as Sum Frequency Generation. Systems of interest range from proteins at water/air interfaces to CO₂ reduction catalysts on electrode surfaces.	
	University of Buenos Aires, Argentina	
	<ul style="list-style-type: none">• Graduate Research Assistant 2012-2016 Advisor: Professor Daniel Laría Research: Investigation of effects derived from the explicit inclusion of nuclear quantum fluctuations upon the structure and dynamics of different aqueous environments, ranging from water clusters at low temperature to condensed phases at ambient conditions.	
TEACHING AND MENTORING EXPERIENCE	Yale University, New Haven, CT	
	Undergraduate and Graduate Student Mentor, Prof. Batista Lab	2016–present
	University of Buenos Aires, Argentina	
	Teaching Assistant, Chemistry Department	2010–2016
	<ul style="list-style-type: none">• Inorganic Chemistry, Lab Class• Physical Chemistry, Lab & Problem Set Class• Statistical Mechanics, Problem Set Class	

AWARDS	Best Poster Award, EMLG/JMLG Annual Meeting, Crete, Greece	2016
	Graduate Fellowship, National Scientific and Technical Research Council (CONICET), Argentina	2012–2016
	Graduation with honors in Chemistry, Medal of Excellence (Dr. Pedro A. Berdoy Award), Argentine Chemical Society (AQA)	2012
	Stimulus Undergraduate Fellowship, University of Buenos Aires, Argentina	2010–2012
OUTREACH ACTIVITIES	University of Buenos Aires, Argentina	
	<i>Chemistry Week</i>	2010-2013
	Design and execution of scientific demonstrations for high school students	
	<i>Night of the Museums</i>	2012
	Design and execution of scientific demonstrations for general public	
	<i>Science Park at ExpoUBA</i>	2010
	Design and execution of scientific demonstrations for general public	
	Argentine Ministry of Science and Technology/Max Planck Society, Argentina	
	<i>The Science Tunnel</i>	2010
	Explanation of chemistry concepts to general public	
JOURNAL REVIEWER	The Journal of Physical Chemistry , American Chemical Society	2018–present
	The Journal of Chemical Physics , American Institute of Physics	2020–present
LANGUAGE PROFICIENCIES	<ul style="list-style-type: none"> • Spanish: Native proficiency. • English: Full professional proficiency. • French: Elementary proficiency. 	
ORAL PRESENTATIONS	<ol style="list-style-type: none"> 1. <i>Characterizing Molecular Systems at Interfaces with SFG</i> Interfacial Molecular and Electronic Structure and Dynamics (virtual conference), Telluride Science Research Center (2020) 2. <i>Nuclear Quantum Effects in Multi-Time Correlation Functions</i> Quantum Effects in Condensed-Phase Systems, Telluride Science Research Center, Telluride, CO (2019) 3. <i>CO₂ Reduction Catalysts on Gold Electrode Surfaces Influenced by Large Electric Fields</i> Solar Meeting, Yale University, New Haven, CT (2019) 4. <i>Floquet Study of Quantum Control of the cis-trans Isomerization of Rhodopsin</i> Connecticut Valley Quantum Chemistry, Yale University, New Haven, CT (2017) 5. <i>Striking Difference Between CO₂ Reduction Catalysts on Nanostructured and Single Crystalline TiO₂ Surfaces</i> Solar Meeting, Yale University, New Haven, CT (2017) 6. <i>Interfacial Structure and Electric Field Probed by in situ Electrochemical Vibrational Stark Effect Spectroscopy and Computational Modeling</i> Solar Meeting, Yale University, New Haven, CT (2017) 	

7. *Nuclear Quantum Effects in Aqueous Clusters at Low Temperatures*
P-Chem Club Seminar, Yale University, New Haven, CT (2016)
8. *Superficial Isotopic Segregation in Aqueous Clusters*
XIX Argentine Congress of Physical and Inorganic Chemistry, Buenos Aires, Argentina (2015)

POSTER
PRESENTATIONS

1. **P. E. Videla**, K. A. Jung, V. S. Batista.
Inclusion of Nuclear Quantum Effects in Multi-Time Correlation Functions
Physics & Chemistry of Water Gordon Research Conferences, Holderness School, NH (2019)
2. **P. E. Videla**, V. S. Batista, E. C. Y. Yan, P. B. Petersen, L. Velarde, T. Lian, C. P. Kubiak.
Theoretical and Experimental Characterization of Catalytic Interfaces Based on SFG and 2D-SFG spectroscopy
Vibrational Spectroscopy Gordon Research Conferences, University of New England, ME (2018)
3. K. A. Jung, **P. E. Videla**, V. S. Batista.
Inclusion of nuclear quantum effects for simulations of nonlinear spectroscopy
Water & Aqueous Solutions Gordon Research Conferences, Holderness School, NH (2018)
4. U. N. Morzan, **P. E. Videla**, E. Nibbering, V. S. Batista.
Pump-Probe UV-Xray: Beyond femtosecond time resolution
Cokerfest (in honor of Prof. David Coker), Boston University, Boston, MA (2018)
5. **P. E. Videla**, P. J. Rossky, D. Laria, V. S. Batista.
Understanding isotopic segregation in aqueous systems
Path Integral Quantum Mechanics School, CECAM-HQ-EPFL, Lausanne, Switzerland (2018)
6. **P. E. Videla**, V. S. Batista.
Quantum Control at a Light-Induced Conical Intersection: Floquet Theory Applied to the Photoisomerization of Rhodopsin
Flatiron CCQ Quantum Chemistry Workshop, New York, NY (2017)
7. **P. E. Videla**, V. S. Batista.
Quantum Control at a Light-Induced Conical Intersection: Floquet Theory Applied to the Photoisomerization of Rhodopsin
American Conference of Theoretical Chemistry, Boston, MA (2017)
8. **P. E. Videla**, A. Ge, G. L. Lee, B. Rudshiteyn, J. Song, C. P. Kubiak, V. S. Batista, T. Lian.
Interfacial Structure and Electric Field Probed by in situ Electrochemical Vibrational Stark Effect Spectroscopy and Computational Modeling
Physics & Chemistry of Water Gordon Research Conferences, Holderness School, NH (2017)
9. **P. E. Videla**, P. Rossky, D. Laría.
Isotope Effects in Aqueous Solvation of Simple Halides
EMLG/JMLG Annual Meeting, Crete, Greece (2016)

10. **P. E. Videla**, P. Rossky, D. Laría.
Isotopic effects on solvation in aqueous clusters
Physics & Chemistry of Water Gordon Research Conferences, Holderness School, NH (2015)
11. **P. E. Videla**, P. Rossky, D. Laría.
Surface isotope segregation as a probe of temperature in water nanoclusters
Water & Aqueous Solutions Gordon Research Conferences, Holderness School, NH (2014)
12. **P. E. Videla**, P. Rossky, D. Laría. *Nuclear quantum effects on the structure and the dynamics of [H₂O]₈ at low temperatures*
Physics & Chemistry of Water Gordon Research Conferences, Holderness School, NH (2013)
13. **P. E. Videla**, Daniel Laría. *Nuclear quantum effects in aqueous clusters at low temperatures*
XVIII Argentine Congress of Physical and Inorganic Chemistry, Rosario, Argentina (2013)
14. **P. E. Videla**, D. Laría.
Aqueous electrolytes confined within silica nanopores
Spring School on Path-Integral Molecular Dynamics, Centre Européen de Calcul Atomique et Moléculaire (CECAM), Toulouse, France (2012)
15. **P. E. Videla**, D. Laría.
Aqueous electrolytes confined within silica nanopores
Structure and Dynamics of Glassy, Supercooled and Nanoconfined Fluids, Buenos Aires, Argentina (2012)
16. **P. E. Videla**, D. Laría.
Aqueous electrolytes confined within silica nanotubes
XVII Argentine Congress of Physical and Inorganic Chemistry, Córdoba, Argentina (2011)
17. **P. E. Videla**, W. S. Shipman, M. B. Rossi, L. M. Baraldo.
Spectroscopic and electrochemical properties of [(DMAP)₄Ru^{II}(μ-NC)Ru^{III}(CN)₅]⁻ in different solvent
XVI Argentine Congress of Physical and Inorganic Chemistry, Salta, Argentina (2009)

JOURNAL
PUBLICATIONS

1. K. A. Jung, **P. E. Videla*** and V. S. Batista.
Ring-Polymer, Centroid and Mean-field Approximations to Multi-time Matsubara Dynamics
accepted in J. Chem. Phys.
*corresponding author
2. U. N. Morzan*†, **P. E. Videla***†, M. B. Soley†, E. T. J. Nibbering and V. S. Batista*.
Vibronic Dynamics of Photodissociating ICN from Simulations of Ultrafast X-Ray Absorption Spectroscopy
Angewandte Chemie DOI: 10.1002/ange.202007192
*corresponding authors
†equal contributions

3. Z. Tong, **P. E. Videla***, K. Jung, V. S. Batista and X. Sun*.
Two-dimensional Raman Spectroscopy of Lennard-Jones Liquids via Ring-Polymer Molecular Dynamics
J. Chem. Phys., 153, 034117 (2020)
*corresponding author
4. M. Cattaneo, F. Guo, H. R. Kelly, **P. E. Videla**, L. Kiefer, S. Gebre, A. Ge, Q. Liu, S. Wu, T. Lian and V. S. Batista.
Robust Binding of Disulfide-Substituted Rhenium Bipyridyl Complexes for CO₂ Reduction on Gold Electrodes
Front. Chem., DOI: 10.3389/fchem.2020.00086
5. K. A. Jung, **P. E. Videla**, V. S. Batista.
Multi-time Formulation of Matsubara Dynamics
J. Chem. Phys., 151, 034108 (2019)
6. E. A. Perets*, **P. E. Videla***, E. C. Y. Yan, V. S. Batista.
Chiral Inversion of Amino Acids in Antiparallel β -Sheets at Interfaces Probed by Vibrational Sum Frequency Generation Spectroscopy
J. Phys. Chem. B, 123, (27) 5769-5781 (2019)
*equal contributions
7. A. Ge*, B. Rudshiteyn*, **P. E. Videla***, C. J. Miller, C. P. Kubiak, V. S. Batista, T. Lian.
Heterogenized Molecular Catalysts: Vibrational Sum-Frequency Spectroscopic, Electrochemical, and Theoretical Investigations
Acc. Chem. Res. 52 (5), 1289-1300 (2019)
*equal contributions
8. M. L. Clark*, A. Ge*, **P. E. Videla***, B. Rudshiteyn, C. J. Miller, J. Song, V. S. Batista, T. Lian, C. P. Kubiak.
CO₂ Reduction Catalysts on Gold Electrode Surfaces Influenced by Large Electric Fields
J. Am. Chem. Soc., 140 (50), 17643-17655 (2018)
*equal contributions
9. H. Vanselous*, **P. E. Videla***, V. S. Batista, P. B. Peterson.
Distinct Binding of Rhenium Catalysts on Nanostructured and Single-Crystalline TiO₂ Surfaces Revealed by Two-Dimensional Sum Frequency Generation Spectroscopy
J. Phys. Chem. C, 122 (45), 26018-26031 (2018)
*equal contributions
10. K. A. Jung, **P. E. Videla***, V. S. Batista*.
Inclusion of Nuclear Quantum Effects for Simulations of Nonlinear Spectroscopy[†]
J. Chem. Phys., 148, 244105 (2018)
*corresponding author
[†]Editor's Pick
11. A. Ge*, **P. E. Videla***, B. Rudshiteyn, Q. Liu, V. S. Batista, T. Lian.
Dopant-Dependent SFG Response of Rhenium CO₂ Reduction Catalysts Chemisorbed on SrTiO₃ (100) Single Crystals
J. Phys. Chem. C 122 (25), 13944-13952 (2018)
*equal contributions
12. **P. E. Videla**, P. J. Rossky, D. H. Laría.
Isotopic Equilibria in Aqueous Clusters at Low Temperatures: Insights from the MB-pol Many-Body Potential
J. Chem. Phys., 148, 084303 (2018)

13. **P. E. Videla**, A. Markmann, V. S. Batista.
Floquet Study of Quantum Control of the cis-trans Photoisomerization of Rhodopsin
J. Chem. Theory Comput., 14(3), 1198-1205 (2018)
14. **P. E. Videla**, P. J. Rossky, D. H. Laría.
Isotope Effects in Aqueous Solvation of Simple Halides
J. Chem. Phys., 148, 102306 (2018)
15. A. Ge*, **P. E. Videla***, G. L. Lee, B. Rudshiteyn, J. Song, C. P. Kubiak, V. S. Batista, T. Lian.
Interfacial Structure and Electric Field Probed by in Situ Electrochemical Vibrational Stark Effect Spectroscopy and Computational Modeling
J. Phys. Chem. A, 121, 18674-18682 (2017)
*equal contributions
16. Y. Guo, H. P. Hendrickson, **P. E. Videla**, Y. Chen, J. Ho, S. Sekharan, V. S. Batista, J. C. Tully, E. C. Y. Yan.
Probing the Remarkable Thermal Kinetics of Visual Rhodopsin with E181Q and S186A Mutants
J. Chem. Phys., 146, 215104 (2017)
17. J. Wang, **P. E. Videla**, V. S. Batista.
Effects of Aligned α -Helix Peptide Dipoles on Experimental Electrostatic Potentials
Prot. Sci., 26, 1692-1697 (2017)
18. **P. E. Videla**, L. Ansourian, D. H. Laría.
Hydrogen Bond Dynamics at Water/Pt Interfaces
J. Phys. Chem. C, 120 (48), 27276-27284 (2016)
19. Y. E. Litman, **P. E. Videla**, J. Rodriguez, D. H. Laría.
Positional Isotope Exchange in $\text{HX}\cdot(\text{H}_2\text{O})_n$ ($X=\text{F},\text{I}$) Clusters at Low Temperatures
J. Phys. Chem. A, 120 (36), 7213-7224 (2016)
20. **P. E. Videla**, P. J. Rossky, D. H. Laría.
Communication: Isotopic Effects on Tunneling Motions in the Water Trimer
J. Chem. Phys., 144, 061101 (2016)
21. **P. E. Videla**, P. J. Rossky, D. H. Laría.
Isotopic Preferential Solvation of I^- in Low-Temperature Water Nanoclusters
J. Phys. Chem. B, 119 (35), 11783-11790 (2015)
22. **P. E. Videla**, P. J. Rossky, D. H. Laría.
Surface Isotope Segregation as a Probe of Temperature in Water Nanoclusters
J. Phys. Chem. Lett., 5 (13), 2375-2379 (2014)
23. **P. E. Videla**, P. J. Rossky, D. H. Laría.
Nuclear Quantum Effects on the Structure and the Dynamics of $[\text{H}_2\text{O}]_8$ at Low Temperatures
J. Chem. Phys., 139 (17), 174315 (2013)
24. **P. E. Videla**, P. J. Rossky, D. H. Laría.
A Quantum Molecular Dynamics Study of Aqueous Solvation Dynamics
J. Chem. Phys., 139 (16), 164506 (2013)
25. **P. E. Videla**, J. Sala, J. Martí, E. Guàrdia, D. H. Laría.
Aqueous Electrolytes Confined Within Functionalized Silica Nanopores
J. Chem. Phys., 135 (10), 104503 (2011)