

# Andrés Montoya-Castillo

University of Colorado Boulder  
Department of Chemistry

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## Career History

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- **Assistant Professor** 2021 – Present  
Department of Chemistry, University of Colorado Boulder, Boulder, CO, 80309
- **Postdoctoral Research Scientist** 2016 – 2020  
Department of Chemistry, Stanford University, Stanford, CA, 94305  
Research advisor: Prof. Thomas E. Markland

## Education

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Degree	Institution	Year
Ph.D., Chemical Physics <i>Advisor: Prof. David R. Reichman</i>	Columbia University	2016
M.Phil., Chemical Physics	Columbia University	2015
M.A., Chemical Physics	Columbia University	2013
B.A., Chemistry & Literature (minor in Physics) <i>Summa cum laude, with departmental and research honors</i>	Macaulay Honors College, CUNY	2009

## Awards

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- Young Faculty Poster Award, Berkeley Statistical Mechanics 2023
- Outstanding poster presentation award, West Coast Theoretical Chemistry Symposium 2018
- Postdoctoral Fellow Award, Penn Conference in Theoretical Chemistry 2017
- Outstanding poster presentation award, American Conference of Theoretical Chemistry 2014
- Graduate School of Arts and Sciences Travel Award, Columbia University 2014
- Jack Miller award for excellence in teaching, Columbia University 2013
- Rutgers Fellowship for academic excellence, Columbia University 2012–2013
- Graduate Faculty Fellowship, Columbia University 2011–2012
- Jerome Schulman award for research in Physical Chemistry, Queens College, CUNY 2009
- Stanley G. Konkol memorial award in Chemistry, Queens College, CUNY 2009

## Teaching & Professional Activities

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- Peer reviewing for: The Journal of Chemical Physics, Journal of Chemical Theory and Computation, Journal of Physical Chemistry A/B, Journal of Physical Chemistry Letters, Physical Chemistry Chemical Physics, Entropy
- Courses at the University of Colorado, Boulder
  - Introductory Quantum Chemistry (graduate) Fall 2021
  - Theoretical & Computational Chemistry (graduate & undergraduate) Spring 2021
- Teaching assistant, Columbia University
  - Graduate Quantum Chemistry Fall 2015
  - General Chemistry I & II Fall 2012 – Spring 2013

– General Chemistry Laboratory

Spring 2012

- Co-Chair, Physical Chemistry Seminar Series, Columbia University Fall 2014 – Spring 2015
- Board member, Physical Chemistry Seminar Series, Columbia University Fall 2011 – Spring 2015
- Lab technician, RFK Science Research Institute Summers, 2005 – 2008

## Invited Lectures

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- [1] *Upcoming*: Berkeley Statistical Mechanics, Berkeley, CA, USA Jan. 2024
- [2] *Upcoming*: ACS National Meeting Symposium: Chemistry and Properties of Two-Dimensional Materials, San Francisco, CA, USA Aug. 2023
- [3] *Upcoming*: ACS National Meeting Symposium: Emerging Techniques to Quantify Biomolecular Conformational Ensembles, San Francisco, CA, USA Aug. 2023
- [4] *Upcoming*: Quantum Effects in Condensed Phase Systems, Telluride, CO, USA Jul. 2023
- [5] *Upcoming*: Exciton Transport in 2D Materials, San Sebastián, Spain Jun. 2023
- [6] *Upcoming*: ACS National Meeting: Symposium on Charge Transfer & Energy Conversion at Interfaces and Defects, Indianapolis, IN, USA Mar. 2023
- [7] Chemistry Department Seminar, Boston University, MA, USA Nov. 2022
- [8] Chemistry Department Seminar, Southern Methodist University, TX, USA Oct. 2022
- [9] Condensed Phase Dynamics, Telluride, CO, USA Jul. 2022
- [10] International Symposium on Molecular Spectroscopy (ISMS), Urbana-Champaign, IL, USA Jun. 2022
- [11] The McGill Molecular Science Mini-Meeting (M&MS), Montreal, Canada Jun. 2022
- [12] Initiative for the Theoretical Sciences (ITS), CUNY Graduate Center, NY, USA May 2022
- [13] Department of Chemistry & Biochemistry, Queens College, CUNY, NY, USA Mar. 2022
- [14] Soft Matter & Biological Physics, Department of Applied Physics, Eindhoven University of Technology, Eindhoven, The Netherlands Mar. 2022
- [15] Center for Synthesizing Quantum Coherence, NSF Center for Chemical Innovation Jan. 2022
- [16] Exciton dynamics in functional materials: New theoretical frontiers, CECAM, Lausanne, Switzerland Dec. 2021
- [17] Quantum Effects in Condensed Phase Systems, Telluride Jun. 2021
- [18] Nonequilibrium dynamical solvent effects on excited states: from spectroscopy to photoreactivity, CECAM, Nancy, France Jun. 2021
- [19] Chemistry Department Seminar, Tel Aviv University, Israel May. 2021
- [20] Theory Journal Club, Chemistry Department, Cornell University April 2021
- [21] ChemBioChem Club, Chemistry Department, University of Colorado, Boulder April 2021
- [22] Chemistry Department Seminar, University of Colorado Boulder Feb. 2020
- [23] Chemistry Department Seminar, Duke University Jan. 2020
- [24] Chemistry Department Seminar, Colorado State University Jan. 2020
- [25] Chemistry Department Seminar, Yale University Jan. 2020
- [26] Chemistry Department Seminar, Texas A&M University Dec. 2019
- [27] Chemistry Department Seminar, Harvard University Nov. 2019
- [28] Tuckerman & Hocky groups, New York University Aug. 2019
- [29] Quantum Effects in Condensed Phase Systems, Telluride Jul. 2019

- [30] Penn Conference in Theoretical Chemistry, University of Pennsylvania  
*Postdoctoral Fellow award* Aug. 2017
- [31] Statistical Mechanics Seminar, UC Berkeley Apr. 2017
- [32] Theory and Applications of Computational Chemistry Conference, Seattle (*contributed*) Sept. 2016

## Scientific Leadership

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- MRS National Meeting, San Francisco April 2022  
*Co-organizer for the Symposium: "2D Materials for Electrochemical Applications — Leading the Charge through Thermodynamic and Kinetic Knowledge Gaps."*
- ACS National Meeting, Indianapolis March 2023  
*Co-organizer for the Symposium: "Experimental and Theoretical Progress in Multidimensional Spectroscopy: Elucidating Charge and Energy Transfer in the Condensed Phase".*

## Synergistic Activities & Outreach

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- Physical Chemistry representative in our first Grad School Virtual Open House Fall 2022  
*Helped plan and execute our department's first Virtual Open House for undergraduates thinking about applying to our graduate program. Announced our efforts through Twitter and the Open House was available to anyone around the world. More than 40 students participated. Answered questions about the program and presented and represented our Physical Chemistry program.*
- GradSchool Readiness BootCamp for incoming Physical Chemistry Graduate Students Summer 2022  
*Started and led the Chemistry Department's first BootCamp program to ensure the readiness of incoming Physical Chemistry graduate students for our graduate program. Developed four learning hubs: computer literacy; statistics; linear algebra; calculus and Fourier transforms. Offered resources to do self-guided learning and illustrative exercises to prepare students for their courses. Concluded with a community-building dinner with faculty members and second-year graduate students to foster collaboration and communication. Provided a leadership and curriculum-building opportunity for current graduate students who led the classes during the BootCamp and wrote about their work in their applications to fellowships: NSF GRFP, the Ford Foundation, and internal grants, such as CU's GAANN program.*
- Justice, Equity, Diversity and Inclusion (JEDI) Committee, CU Boulder Chemistry 2022 – Present  
*Spearheaded and co-chaired (2022) the JEDI committee in the chemistry department at CU Boulder. We founded the JEDI committee to foster a more inclusive and encouraging environment in the chemistry department for all its members and to help ensure the welfare of graduate students.*
- Consulting research scientist and mentor, RFK Science Research Institute (RFKSRI) 2011/2016 – Present  
*Serve as scientific advisor (2016 – Present) and mentor (2011 – Present) at the RFKSRI, a highly selective program that provides high school and undergraduate students, especially those from underrepresented groups like women and minorities from New York City area, an opportunity to do science research in geochemistry, archaeology, and paleoanthropology to develop their critical thinking, logical reasoning, scientific writing and presentation skills. As part of this program, I have mentored more than 20 students over the past decade.*
- Mentor in the Out in Science, Technology, Engineering, & Mathematics (oSTEM), Stanford University 2016 – 2017  
*Served as an informal mentor to one master's (now Ph.D.) student in biophysics through the oSTEM mentoring program, a national student society, dedicated to increasing the participation of queer people in disciplines related to science, technology, engineering, or mathematics.*
- Alumni representative in Student Life Committee, Macaulay Honors College 2014 – 2016

*Represented the interests of the student community, interacting frequently with the previous and current deans, Prof. Ann Kirschner and Prof. Mary Pearl, advocating for mental health resources, and serving as an alumnus ambassador during a Sloan Foundation pitch.*

- Mentor in the Macaulay Mentors Program, Macaulay Honors College 2014 – 2016

*Mentored three undergraduate students, helping them navigate internship, graduate school, and medical school application processes, providing support as they designed their Bachelor's theses and worked to complete them.*

- Judge, New York City Science and Engineering Fair (NYCSEF) 2013 – 2016

*Served as judge the initial and final rounds of the chemistry, physics, and earth science categories at NYCSEF for three years. Having competed in this program as a high school student, I brought my appreciation of the hard work high school students invest into their projects to not only assess their scientific thinking and creativity, but also encourage them to continue pursuing their passion for science.*

## Publications

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- [1] A. J. Dominic, S. Cao, **A. Montoya-Castillo**, X. Huang. “Memory unlocks the future of biomolecular dynamics: Transformative tools to uncover physical insights accurately and efficiently.” ChemRxiv:10.26434/chemrxiv-2023-920jj (2023)
  - [2] **A. Montoya-Castillo**, T. E. Markland. “A derivation of the conditions under which bosonic operators exactly capture fermionic structure and dynamics.” arXiv:2212.07003 (2022)
  - [3] A. O. Atsango, **A. Montoya-Castillo**, T. E. Markland. “An accurate and efficient Ehrenfest dynamics approach for calculating linear and nonlinear electronic spectra.” arXiv:2212.06973 (2022) [*Just accepted at J. Chem. Phys.*]
  - [4] A. J. Dominic, T. Sayer, S. Cao, T. E. Markland, X. Huang, **A. Montoya-Castillo**. “Building insightful, memory-enriched models to capture long-time biochemical processes from short-time simulations.” biorXiv: 2022.10.17.512620 (2022) [*Just accepted at the Proc. Nat. Acad. Sci.*]
  - [5] R. Austin, Y. R. Farah, T. Sayer, B. M. Luther, **A. Montoya-Castillo**, A. T. Krummel, J. B. Sambur. “Hot carrier extraction from 2D semiconductor photoelectrodes.” arXiv:2210.13588 (2022) [*Just accepted at the Proc. Nat. Acad. Sci.*]
  - [6] A. Vezvaei, N. Shitara, S. Sun, **A. Montoya-Castillo**. “Noise Spectroscopy Without Dynamical Decoupling Pulses.” arXiv:2210.00386 (2022)
  - [7] T. Sayer, **A. Montoya-Castillo**. “Compact and complete description of non-Markovian dynamics.” J. Chem. Phys. **158**, 014105 (2023) — *Selected as an Editor’s Pick by the Journal of Chemical Physics.*
  - [8] **A. Montoya-Castillo**, M. S. Chen, S. L. Raj, K. A. Jung, K. S. Kjaer, T. Morawietz, K. J. Gaffney, T. B. van Driel, T. E. Markland. “Optically induced anisotropy in time-resolved scattering: Imaging molecular scale structure and dynamics in disordered media with experiment and theory.” Phys. Rev. Lett. **129**, 056001. (2022)
- Before starting at the University of Colorado Boulder
- [9] Y. Mao, **A. Montoya-Castillo**, T. E. Markland. “Excited state diabaticization on the cheap using DFT: Photoinduced electron and hole transfer.” J. Chem. Phys. **153**, 244111. (2020)
  - [10] S. Cao, **A. Montoya-Castillo**, W. Wang, T. E. Markland, X. Huang. “On the advantages of exploiting memory in Markov state models for biomolecular dynamics.” J. Chem. Phys. **153**, 014105. (2020)
  - [11] Y. Mao, **A. Montoya-Castillo**, T. E. Markland. “Accurate and efficient DFT-based diabaticization for hole and electron transfer using absolutely localized molecular orbitals.” J. Chem. Phys. **151**, 164114. (2019)
  - [12] T. J. Zuehlsdorff<sup>†</sup>, **A. Montoya-Castillo**<sup>†</sup>, J. A. Napoli, T. E. Markland, C. M. Isborn. “Optical spectra in the condensed phase: Capturing anharmonic and vibronic features using dynamic and static approaches.” J. Chem. Phys. **151**, 074111. (2019)
  - [13] W. C. Pfalzgraff, **A. Montoya-Castillo**, A. Kelly, T. E. Markland. “Efficient construction of generalized master equation memory kernels for multi-state systems from nonadiabatic quantum-classical dynamics.” J. Chem. Phys. **150**, 244109. (2019)

- [14] **A. Montoya-Castillo**, T. E. Markland. “On the exact continuous mapping of fermions.” *Sci. Rep.* **8**, 12929. (2018)
- [15] **A. Montoya-Castillo**, D. R. Reichman. “Approximate but accurate dynamics from the Mori formalism: II. Equilibrium correlation functions.” *J. Chem. Phys.* **146**, 084110. (2017)
- [16] **A. Montoya-Castillo**, D. R. Reichman. “Path integral approach to the Wigner representation of canonical density operators for discrete systems coupled to harmonic baths.” *J. Chem. Phys.* **146**, 024107. (2017)
- [17] A. Kelly<sup>†</sup>, **A. Montoya-Castillo**<sup>†</sup>, L. Wang, T. E. Markland. “Generalized quantum master equations in and out of equilibrium: How can one win?” *J. Chem. Phys.* **144**, 184105. (2016)
- [18] **A. Montoya-Castillo**, D. R. Reichman. “Approximate but accurate dynamics from the Mori formalism: I. Nonequilibrium dynamics.” *J. Chem. Phys.* **144**, 184104. (2016)
- [19] A. Raja, **A. Montoya-Castillo**<sup>†</sup>, J. Zultak<sup>†</sup>, X.-X. Zhang, Z. Ye, C. Roquelet, D. A. Chenet, A. M. van der Zande, P. Huang, S. Jockusch, J. Hone, D. R. Reichman, L. E. Brus, T. F. Heinz. “Energy transfer from quantum dots to graphene and MoS<sub>2</sub>: screening vs. absorption.” *Nano Lett.* **16**, 2328. (2016)
- [20] B. A. B. Blackwell, A. R. Skinner, J. I. B. Blickstein, **A. C. Montoya**, J. A. Florentin, S. M. Baboumian, I. J. Ahmed, A. E. Deely. “ESR in the 21st century: From buried valleys and deserts to the deep ocean and tectonic uplift.” *Earth-Sci. Rev.* **158**, 125. (2016)
- [21] **A. Montoya-Castillo**, T. C. Berkelbach, D. R. Reichman. “Extending the applicability of Redfield theories into highly non-Markovian regimes.” *J. Chem. Phys.* **143**, 194108. (2015)
- [22] S. Jang, **A. Montoya-Castillo**. “Charge hopping dynamics along a disordered chain in quantum environments: Comparative study of different rate kernels.” *J. Phys. Chem. B.* **119**, 7659. (2015)
- [23] B. A. B. Blackwell, **A. Montoya**, J. I. B. Blickstein, A. R. Skinner, S. Pappu, Y. Gunnell, M. Taieb, A. Kumar, J. A. Lundberg. “ESR analyses for teeth from the open-air site at Attirampakkam, India: Clues to complex U uptake and paleoenvironmental change.” *Radiat. Meas.* **42**, 1243. (2007)

<sup>†</sup> denotes equal author contribution