

Daniel G. Kuroda, Ph.D.

Associate Professor of Chemistry, Louisiana State University

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EDUCATION

B.S. Chemistry - *University of Buenos Aires* (UBA), Argentina. April 2002

Undergraduate Research Director - Prof. Ernesto Marceca

Research Topic - Study of Ion-molecule Atmospheric Reactions by Mass Spectrometry

Ph.D. Chemistry - *University of Florida*, Gainesville, Florida, May 2008

Ph.D. Advisor - Prof. Valeria D. Kleiman

Thesis: *"In the quest of manipulating light-matter interactions: Coherent control of two photon induced processes in solution."*

PROFESSIONAL EXPERIENCE

2019-pres. Associate Professor, Louisiana State University, Baton Rouge, Louisiana.

2013-2019 Assistant Professor, Louisiana State University, Baton Rouge, Louisiana.

2008-2013 Postdoctoral Associate, Department of Chemistry, University of Pennsylvania, Philadelphia, Pennsylvania (August 2008- July 2013).

Postdoctoral Research Advisor: Prof. Robin M. Hochstrasser (deceased).

2012- 2013 Consultant for Adesys, Inc.

1999-2000 Laboratory Technician, INQUIMAE, School of Science, University of Buenos Aires, Argentina.

1999-2000 High School Teacher, Philips Argentina Technical High School, Buenos Aires, Argentina.

HONORS AND AWARDS**- At Louisiana State University**

2018 National Science Foundation CAREER award.

2018 Tiger Athletic Foundation College Undergraduate Teaching Award.

2017 LSU Alumni Association Rising Faculty Research Award.

2014 Fellow of the National Academy of Education in Science 2014-2015.

- At University of Florida

2007 Student Travel Grant Award. APS, Frontiers in Optics 2007 - Laser Science XXIII, San Jose, CA.

2006 Physical Chemistry Student Poster Award. ACS, 231st National Meeting, Atlanta, Ga.

- 2005 Teaching award. Physical Chemistry Division, Department of Chemistry, University of Florida.
- 2005 Proctor & Gamble Research Award for excellence in graduate research. Department of Chemistry, University of Florida.

- At University of Buenos Aires

- 2000 University of Buenos Aires scholarship (BECA UBA) for undergraduate research. Universidad the Buenos Aires. Buenos Aires Argentina.

Scholarship

Shorter works

- Chapters in books

1. Polarization anisotropy effects for degenerate vibrational levels, book chapter in Ultrafast Infrared Vibrational Spectroscopy, Kuroda DG, Hochstrasser RM. Editor: Michael D. Fayer. CRC Press, 2013, ISBN: 1466510137.

- Articles in refereed journals

Peer-Reviewed Publications (from independent research at LSU and * is corresponding author)

1. Sepulveda-Montañó LX, Galindo JF, & Kuroda DG. "Infrared Spectroscopy of Liquid Solutions as a Benchmarking Tool of Semiempirical QM Methods: The Case of GFN2-xTB." The Journal of Physical Chemistry B, 2023, 127, 7955-7963.
2. Gurung A & Kuroda DG*. "A new method based on pseudo-Zernike polynomials to analyze and extract dynamical and spectral information from the 2DIR spectra." The Journal of Chemical Physics, 2023, 159, 034201 (2023).
3. Rushing JC, Gurung A & Kuroda DG*. "Relation between microscopic structure and macroscopic properties in polyacrylonitrile-based lithium-ion polymer gel electrolytes." The Journal of Chemical Physics, 2023, 158, 144705.
4. Chen X & Kuroda DG*. "Ionic Conduction Mechanism in High Concentration Lithium Ion Electrolytes." Chemical Communications, 2023, 59, 1849-1852
5. Nachaki EO, Leonik FM & Kuroda DG*. "Effect of the N-Alkyl Side Chain on the Amide–Water Interactions." The Journal of Physical Chemistry B, 2022, 126, 8290-8299.
6. Zhang X, Zhou S, Leonik FM, Wang L, & Kuroda DG*. "Quantum mechanical effects in acid–base chemistry." Chemical science, 2022, 13, 6998-7006.
7. Pestana-Nobles R, Aranguren-Díaz Y, Machado-Sierra E, Yosa J, Galan-Freyle NJ, Sepulveda-Montañó LX, Kuroda DG, Pacheco-Londoño LC. "Docking and Molecular Dynamic of Microalgae Compounds as Potential Inhibitors of Beta-Lactamase." International Journal of Molecular Sciences, 2022, 23, 3, 1630.
8. Rushing JC, Stern CM, Elgrishi N, Kuroda DG*. "Tale of a "Non-interacting" Additive in a Lithium-Ion Electrolyte: Effect on Ionic Speciation and Electrochemical Properties." The Journal of Physical Chemistry C, 2022, 126, 4, 2141-2150.

9. Cui Y, Rushing JC, Seifert S, Bedford NM, Kuroda DG*, "Structural and dynamical changes observed when transitioning from an ionic liquid to a deep eutectic solvent." *The Journal of Chemical Physics*, 2021, 155, 5, 054507.
10. Fulfer KD, Galle Kankanamge SR, Chen X, Woodard KT, Kuroda DG*. "Elucidating the mechanism behind the infrared spectral features and dynamics observed in the carbonyl stretch region of organic carbonates interacting with lithium ions." *The Journal of Chemical Physics*, 2021, 154, 23, 234504.
11. Zhang X, Chen X, Kuroda DG*, "Computing the frequency fluctuation dynamics of highly coupled vibrational transitions using neural networks", *The Journal of Chemical Physics*, 2021, 154, 16, 164514.
12. Gobeze HB, Ma J, Leonik FM and Kuroda DG*, "Bottom-Up Approach to Assess the Molecular Structure of Aqueous Poly (N-Isopropylacrylamide) at Room Temperature via Infrared Spectroscopy", *The Journal of Physical Chemistry B*, 2020, 51, 11699–11710
13. Chen X and Kuroda DG*, "Molecular motions of acetonitrile molecules in the solvation shell of lithium ions" *The Journal of Chemical Physics* 2020, 16, 164502.
14. Galle Kankanamge SR, Ma J, Mackin RT, Leonik FM, Taylor CM, Rubtsov IV, Kuroda DG*, "Proving and Probing the Presence of the Elusive CH \cdots O Hydrogen Bond in Liquid Solutions at Room Temperature", *Angewandte Chemie (International ed. in English)*, 2020, 59, 17012-17017.
15. Chen X, Cui Y, Gobeze HB, Kuroda DG*, "Assessing the Location of Ionic and Molecular Solutes in a Molecularly Heterogeneous and Nonionic Deep Eutectic Solvent", *The Journal of Physical Chemistry B*, 2020, 124, 4762–4773.
16. Galle Kankanamge SR, Kuroda DG*, "Molecular Structure, Chemical Exchange, and Conductivity Mechanism of High Concentration LiTFSI Electrolytes" *The Journal of Physical Chemistry B*, 124, 1965-1977.
17. Chen X, Fulfer KD, Woodard KT, Kuroda DG*, "Structure and Dynamics of the Lithium Ion Solvation Shell in Ureas", *Journal of Physical Chemistry B*. 2019, 123, 9889-9898.
18. Rushing JC, Leonik FM, and Kuroda DG*, "Effect of Solvation Shell Structure and Composition on Ion Pair Formation: The Case Study of LiTDI in Organic Carbonates ", *Journal of Physical Chemistry C*, 2019, 123, 25102-25112.
19. Cui Y, Rushing JC, Seifert S, Bedford NM, and Kuroda DG*, "Molecularly Heterogeneous Structure of a Nonionic Deep Eutectic Solvent Composed of N-Methylacetamide and Lauric Acid", *Journal of Physical Chemistry B* 2019, 123, 3984-3993.
20. Zhang X, Kuroda DG*, "An ab initio molecular dynamics study of the solvation structure and ultrafast dynamics of lithium salts in organic carbonates: A comparison between linear and cyclic carbonates", *Journal of Chemical Physics*, 2019, 150, 184501.
21. Galle Kankanamge SR, Kuroda DG*, "Molecular structure and ultrafast dynamics of sodium thiocyanate ion pairs formed in glymes of different lengths", *Physical Chemistry Chemical Physics*, 2019, 21, 833-841.

22. Galle Kankanamge SR, Li K, Fulfer KD, Du P, Jorn R, Kumar R, Kuroda DG*, "Mechanism behind the Unusually High Conductivities of High Concentrated Sodium Ion Glyme-Based Electrolytes", *Journal of Physical Chemistry C*, 2018, 122, 25237-25246.
23. Fulfer KD, Kuroda DG*, "Ion Speciation of Lithium Hexafluorophosphate in Dimethyl Carbonate Solutions: An Infrared Spectroscopy Study", *Physical Chemistry Chemical Physics*, 2018, 22710-22718.
24. Zhang X, Kuroda DG*, "Acetate Ion and its Interesting Solvation Shell Structure and Dynamics", *Journal of Chemical Physics*, 2018, 148, 094506.
25. Li K, Galle Kankanamge SR, Weldeghiorghis TK, Jorn R, Kuroda DG and Kumar R, "Predicting Ion Association in Sodium Electrolytes: A Transferrable Model for Investigating Glymes," *Journal of Physical Chemistry C*, 2018, 122, 4747-4756. FRONT COVER ARTICLE
26. Cui Y and Kuroda DG*, "Evidence of Molecular Heterogeneities in Amide Based Deep Eutectic Solvents", *Journal of Physical Chemistry A*, 2018, 122, 1185-1193. (Invited, Special Issue: Time Resolved Vibrational Spectroscopy).
27. Cui Y, Li MC, Wu Q, Pojman JA, Kuroda DG*, "Synthesis-Free Phase-Selective Gelator for Oil-Spill Remediation", *ACS Applied Materials & Interfaces*, 2017, 9, 33549-33553.
28. Fulfer KD, Kuroda DG*, "A comparison of the solvation structure and dynamics of the lithium ion in linear organic carbonates with different alkyl chain lengths", *Physical Chemistry Chemical Physics*, 2017, 19, 25140-25150.
29. Devereux CJ, Fulfer KD, Zhang X, Kuroda DG*, "Vibrational spectroscopy modeling of a drug in molecular solvents and enzymes", *Chemical Physics*, 2017, 495, 1-9.
30. Ma J, Xuan S, Guerin AA, Yu T, Zhang D, Kuroda DG*, "Unusual molecular mechanism behind the thermal response of polypeptoids in aqueous solutions", *Physical Chemistry Chemical Physics*, 2017, 19, 10878-10888.
31. Cui Y, Fulfer KD, Ma J, Weldeghiorghis TK, Kuroda DG*, "Solvation Dynamics of an Ionic Probed in Choline Chloride-based Deep Eutectic Solvent", *Physical Chemistry Chemical Physics*, 2016, 18, 31471-31479.
32. Fulfer KD, Kuroda DG*, "Solvation Structure and Dynamics of the Lithium Ion in Organic Carbonate-Based Electrolytes: A Time-Dependent Infrared Spectroscopy Study", *Journal of Physical Chemistry C*, 2016, 120, 24011-24022.
33. Wahlers J, Fulfer KD, Harding DP, Kuroda DG*, Kumar R, Jorn R, "Solvation Structure and Concentration in Glyme-Based Sodium Electrolytes: A Combined Spectroscopic and Computational Study". *Journal of Physical Chemistry C*, 2016, 120, 17949-17959.
34. Guerin AC, Riley K, Rupnik K, Kuroda DG*, "Determining the Energetics of the Hydrogen Bond through FTIR: A Hands-On Physical Chemistry Lab Experiment", *Journal of Chemical Education*, *J. Chem. Educ.*, 2016, 93, 1124-1129.
35. Galindo JF, Atas E, Altan A, Kuroda DG, Fernandez-Alberti S, Tretiak S, Roitberg AE, Kleiman VD, "Dynamics of Energy Transfer in a Conjugated Dendrimer Driven by Ultrafast

Localization of Excitations”, J. Am. Chem. Soc., 2015, 137, 11637-11644. FRONT COVER ARTICLE.

36. Li T, Cui Y, Mathaga J, Kumar R, Kuroda DG*, “Hydration and vibrational dynamics of betaine (N,N,N-trimethylglycine)”, Journal of Chemical Physics, 2015, J. Chem. Phys., 2015, 142, 212438. (Invited, Special topic: Multidimensional Spectroscopy)
37. Chuntanov L, Kumar R, Kuroda DG*, “Non-linear infrared spectroscopy of the water bending mode: Direct experimental evidence of hydration shell reorganization?”, Physical Chemistry Chemical Physics, 2014,16, 13172-13181.

Peer-Reviewed Publications (from research before LSU appointment)

38. Kuroda DG*, Abdo M, Chuntanov L, Smith AB, III, Hochstrasser RM, “Vibrational dynamics of a non-degenerate ultrafast rotor: the (C12,C13)-oxalate ion”, Journal of Chemical Physics, 2013, 139, 164514.
39. Singh PK, Kuroda DG*, Hochstrasser RM, “An Ion’s Perspective on the Molecular Motions of Nanoconfined Water: A Two-Dimensional Infrared Spectroscopy Study”, Journal of Physical Chemistry B, 2013, 117, 9775–9784.
40. Chuntanov L, Kuroda DG, Ghosh A, Ma J, Hochstrasser RM, “Quantum beats and coherence decay in degenerate states split by solvation”, Journal of Physical Chemistry Letters, 2013, 4 , 1866–1871.
41. Kuroda DG, Bauman JD, Challa JR, Patel D, Troxler T, Das K, Arnold E, Hochstrasser RM, “Snapshot of the equilibrium dynamics of a drug bound to HIV-1 reverse transcriptase”, Nature Chemistry, 2013, 5, 174–181. FRONT COVER ARTICLE
42. Kuroda DG, Singh PK, Hochstrasser RM, “Differential Hydration of Tricyanomethanide Observed by Time Resolved Vibrational Spectroscopy”, Journal of Physical Chemistry B, 2013, 117, 4354–4364.
43. Kuroda DG, Hochstrasser RM, “Dynamic structures of aqueous oxalate and the effects of counterions seen by 2D IR”, Physical Chemistry Chemical Physics, 2012, 14, 6219-6224.
44. Kuroda DG, Hochstrasser RM, “2D IR spectral signature and hydration of the oxalate dianion”, Journal of Chemical Physics, 2011, 135, 204502.
45. Kuroda DG, Singh CP, Peng ZH, and Kleiman VD. “Exploring the role of phase modulation on photoluminescence yield”. Faraday Discussions, 2011, 153, 61-72.
46. Vorobyev DY, Kuo CH, Kuroda DG, Scott JN, Vanderkooi JM, Hochstrasser RM. “Water-Induced Relaxation of a Degenerate Vibration of Guanidium Using 2D IR Echo Spectroscopy”. Journal of Physical Chemistry B, 2010, 114, 8, 2944-2953.
47. Kuroda, DG; Vorobyev, DY; Hochstrasser, RM. “Ultrafast relaxation and 2D IR of the aqueous trifluorocarboxylate ion”. Journal of Chemical Physics, 2010, 132, 4, 044501. FRONT COVER ARTICLE
48. Vorobyev DY, Kuo CH, Chen JX, Kuroda DG, Scott JN, Vanderkooi JM, Hochstrasser RM. “Ultrafast Vibrational Spectroscopy of a Degenerate Mode of Guanidinium Chloride“. Journal of Physical Chemistry B, 2009, 113, 46, 15382-15391.

49. Kuroda DG, Singh CP, Peng ZH, Kleiman VD. "Mapping Excited-State Dynamics by Coherent Control of a Dendrimer's Photoemission Efficiency". *SCIENCE*, 2009, 326, 5950, 263-267.
50. Kuroda DG, Kleiman VD "Quantum Control of Two-Photon Fluorescence in Solution". Eds.: R. J. D. Miller, A. M. Weiner, P. Corkum, D. M. Jonas, Springer Series in Chemical Physics, Vol 88 (Springer Berlin), 2007. ISBN: 978-3-540-68779-5.

- ***Conference Proceedings (not reviewed)***

1. Fulfer KD, Kuroda DG*, "Molecular Motions, Structure, and Composition of Carbonates in the Solvation Shell of the Lithium Ion, Via Infrared Spectroscopies", *ECS Trans.*, 2017, 77, 1, 3-10.
2. Woodard KT, Fulfer KD, Kuroda DG*, "Exploring the Energetics of the Lithium Ion-Organic Carbonate Interaction: A FTIR and DFT Study", *ECS Trans.*, 2017, 77, 1911-1917.
3. Fulfer KD, Kuroda DG*, "Characterizing the Effects of the Alkyl Chain Length of Linear Organic Carbonates on Lithium Ion Electrolyte Structure and Dynamics: A Solvent Perspective", *ECS Trans.*, 2017, 77, 47-53.

- ***Intellectual Property***

1. Kuroda, Daniel, Kristen Fulfer, and Kaylee Theresa Woodard. "Amide-based electrolyte battery." U.S. Patent No. 11,367,904. 21 Jun. 2022.
2. Kuroda, Daniel, Kristen Fulfer, and Kaylee Theresa Woodard. "Amide-based electrolyte battery." U.S. Patent No. 10,797,351. 6 Oct. 2020.

- ***Media Appearances and Interviews***

1. Interviewed by ScienceNews, September 2015.
(<https://www.sciencenews.org/article/elusiveacid-finally-created>)
2. Interview by ChemistryWorld, June 2022.
(<https://www.chemistryworld.com/news/quantum-nature-of-hydrogen-bonds-observed-in-acid-base-complex/4015766.article>)

Theses / dissertations directed at LSU

- ***Postdoctoral Associate***

Orlando Carrillo Bohorquez, Ph.D., Universidad Nacional de Bogota, Colombia	October 2022 - present
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- ***Ph.D. Students***

Ernest Nachaki, B.S., Kenyatta University, Kenya	Fall 2019 - present
Ani Gurun, MSc., Idaho State University	Fall 2020 - present
Laura Sepulveda, B.S., Universidad Nacional de Bogota, Colombia	Spring 2021 - present

- ***Undergraduate Students***

Amelia Skinner, pursuing BS Chemistry,

Fall 2022 – present

Parquet Collet, pursuing BS Chemistry

Spring 2023 – present

Former Group Members

- Ph.D. Recipients

Jeramie Rushing, B.S., University of Alabama, (fall 2016 – spring 2022), Dissertation Defense: 01/26/2022.

Xiaobing Chen, B.S. Qingdao University of Science & Technology, China (fall 2016 - spring 2021), Dissertation Defense: 05/06/2021.

Susith R Galle Kankanamge, B.S., University of Colombo, Sri Lanka (fall 2015 - spring 2021), Dissertation Defense: 12/03/2020.

Xiaoliu Zhang, B.S., University of Science & Technology of China (fall 2014 - spring 2020), Dissertation Defense: 03/30/2020.

Yaowen Cui, M.S., University of Kentucky (fall 2013 - summer 2018), Dissertation Defense: 04/19/2018.

- M.S. Recipients

Jianbo Ma, B.E., Wuhan Institute of Technology – China (fall 2013 - summer 2017), Thesis Defense: 06/06/2017

- Former Postdoctoral Associate

Juriti Rajbangshi, Ph.D. Chemistry, S. N. Bose National Centre for Basic Sciences, Kolkata, India, (Spring 2022 – Summer 2022), currently postdoctoral research University of Wisconsin, Madison, Wisconsin.

Habtom Gobeze, Ph.D. Chemistry, University of North Texas (Fall 2019 - Fall 2020), currently postdoctoral research University of Texas, San Antonio, Texas.

Kristen Fulfer, Ph.D. Chemistry, Louisiana State University (fall 2015 - summer 2017), currently Assistant Professor, Department of Chemistry, Centre College, Danville, Kentucky

- Former Undergraduates

Christian Foti, BS Chemistry, spring 2023.

Maya Billiot, BS Chemistry, summer 2021 – summer 2022.

Kathia Perez, BS Chemistry, spring 2022.

Jhacory T Simien, spring 2018.

Kaylee Woodard, BS Chemistry (Spring 2017), spring 2015 - summer 2017.

Ashton Avery, BS Biochemistry (Summer 2017), spring 2017 - summer 2017.

Mark Emerson, BS Chemistry (Spring 2017), spring 2017.

Kristi D. Riley, BS Chemistry (December 2014), summer 2014 - fall 2014.

Abby Guerin, BS Chemistry (Spring 2016), fall 2014 - fall 2015.

Christian Devereux, BS Chemistry (Spring 2016), fall 2014 - summer 2016.

Professional service***Advisory boards, commission or agencies***

Served as vice-chair, Chair-elect, Chair and past-Chair in the Experimental subdivision of the ACS PHYS division (Spring 2019 - present)

Reviewing of proposals and manuscripts

Proposal

Department of Energy; Army Research Office; Air Force Office of Scientific Research; ACS-Petroleum Research Fund; National Science Foundation

Journals

Analyst; Analytical Chemistry; Applied Physics Letters; Biomacromolecules; Chemistry - A European Journal; Chemical Physics; Chemical Reviews; Nature; Communications; Physical Chemistry Chemical Physics; Journal of the American Chemical Society; The Journal of Chemical Physics; The Journal of Physical Chemistry A,B,C; The Journal of Physical Chemistry Letters; The Journal of Chemical Education; Journal of The Electrochemical Society; Proceedings of the National Academy of Sciences; RCS Advances; Scientific Reports

Other external service

- Organizer and presenter in the Second grade class of the Baton Rouge Foreign Language Academic Immersion Magnet elementary School, May 2022
- Presenter in the Baton Rouge Shell 4th Energy Camp, July 2016.
- Presenter for the outreach program Speaking of Science organized by the Louisiana Board of Regents (2017 - present)
- Organizer of the outreach program, "The LSU experience" designed at bringing high-school students to LSU before they go to college, 2017-present.
- Organizer and presenter a booth displaying Electrochemical conversion with Dr. Elgrishi for LSU's Superscience Saturday 2019 and 2023.
- Presenter in the LSU environmentors program, which is an award winning after-school science mentoring initiative that pairs underserved high school students from Scotlandville Magnet High with LSU graduates and undergraduates, March 2019.