•	o-Hernández, Ph.D. leserve University chemistry	
	-	one: (216)-368-1911
		nail: carlos.crespo@case.edu
http://orcid.or	rg/0000-0002-3594-0890	
Google Scholar I	-	
Professional	Visiting Professor	2006 – 2007
Preparation	University of Puerto Rico, Humacao Campus, Puerto Rico Research work with A. E. Alegría on Photochemical Investigations of Research and Quineae Carborners with DNA	f
	Pheophorbide-a and Quinone Carboquone with DNA Research Associate	2005 – 2006
	The Ohio State University, Columbus, OH	2003 – 2000
	Research work with B. Kohler on Ultrafast Excited State Dynamics ir and Double-Stranded DNA Polymers	n Single-
	NIH Postdoctoral Fellow	2003 – 2005
	The Ohio State University, Columbus, OH	
	Research work with B. Kohler on Ultrafast Excited State Dynamics in Nucleic Acids	
	Ph.D. in Physical Chemistry	2002
	University of Puerto Rico, San Juan Campus, Puerto Rico Graduate work with R. Arce on Photophysical and Photochemical Str in Nucleic Acids	udies
	B.S. in Chemistry	1995
	University of Puerto Rico, San Juan Campus, Puerto Rico	1000
	Research work with R. Arce on Photochemistry of DNA and Amino A Components	cid
Appointments	Associate Dean for Research,	2021 – present
	College of Arts and Sciences,	
	Case Western Reserve University, Cleveland, OH	
	Associate Member, Case Comprehensive Cancer Center	2021 – present
	Professor	2019 – present
	Case Western Reserve University, Cleveland, OH	
	Associate Professor	2014 – 2019
	Case Western Reserve University, Cleveland, OH	
	Co-director of the Center for Chemical Dynamics	2008 – 2018
	Case Western Reserve University, Cleveland, OH	
	Graduate Faculty of Civil, Environmental and Architectural Engi	neering 2012 – 2015
	External Thesis Committee, University of Colorado, Boulder, Co	
	Frank Hovorka Assistant Professorship in Chemistry	2012 – 2014
	Case Western Reserve University, Cleveland, OH	
	Assistant Professor	2007 – 2014
	Case Western Reserve University, Cleveland, OH	

# Membership in Professional Societies

- 1) American Chemical Society
- 2) American Chemical Society, Physical Chemistry Division
- 3) American Society for Photobiology
- 4) Inter-American Photochemical Society
- 5) Royal Society of Chemistry

# Honors and Awards

- 1) Member of Institute for Smart, Secure and Connected Systems Internal Advisory Board, Case Western Reserve University (2022 present).
- 2) Member of the Scientific Revision Board of the Puerto Rico Science, Technology and Research Trust (2022 present).
- Plenary Speaker at the 40<sup>th</sup> Puerto Rico Interdisciplinary Scientific Meeting (PRISM) and 55<sup>th</sup> American Chemical Society Junior Technical Meeting, University of Puerto Rico, Humacao Campus, Humacao, Puerto Rico, April 9, 2022.
- 4) Nominated for the 2022 John S. Diekhoff Award for Distinguished Graduate Mentoring, Case Western Reserve University (2022).
- 5) Selected as a 2021 Mentor Fellows, Case Western Reserve University.
- 6) Selected as a 2020 STAIR Mentor Fellows Program, Case Western Reserve University.
- 7) Selected for the first cohort of the <u>100+ Latinos Cleveland Must Know</u>, Cleveland, Ohio, 2020.
- 8) Member of the 2020 Committees of Visitors (COVs) at the National Science Foundation.
- 9) Selected as a member of the American Chemical Society Selection Committee for the Ahmed Zewail Award in Ultrafast Science and Technology (2020, 2021, & 2022).
- 10) Invited lecture and Award Presentation at the 5<sup>th</sup> Annual Targeting Excellence: Hispanic Latino Student Initiative, Talk: "DNA + Light: From Intrinsic Photostability of Nucleic Acid bases to Modifications that Facilitate Damage to Skin Cancer Cells", Department of Chemistry, University of Louisville, Louisville, Kentucky, February 22, 2019. Previous invited speakers: Eloy Rodríguez (Cornell), Rigoberto Hernández (Johns Hopkins), Miguel García Garibay (UCLA), Luis Echegoyen (UTEP), Alan Aspuru-Guzik (Harvard), Tomas Kirchhausen (Harvard Medical School), Patricia Dos Santos (Wake Forest), Carlos Correia (Unicamp, Brasil), Luis Campos (Columbia), Héctor Abruña (Cornell) and José Carlos Aponte (NASA).
- 11) Nominated for the 2018 John S. Diekhoff Award for Distinguished Graduate Student Teaching, Case Western Reserve University (2018).
- 12) Invited panelist, featured as a 'Journey (teller)', for the 2018 Reaction Mechanisms Conference: Diversity Symposium, "Journey (tellers): Thrive, Survive Stories: Diversity Edition", University of British Columbia, Vancouver, Canada, (2018).
- One of 13 faculty members selected to mentor undergraduate students in chemistry and the biological sciences for the prestigious Arnold and Mabel Beckman Foundation Scholars Awards Program at CWRU (2018 – 2020).
- 14) 2017 Morton L. Mandel Award. Awarded annually to a member of the faculty of the CWRU Department of Chemistry to recognize excellence in the department through their research, teaching, mentoring or service.
- 15) Chair of the American Chemical Society <u>Canvassing Committee for the Ahmed Zewail Award in Ultrafast</u> <u>Science and Technology</u> (2016 – 2019).
- 16) Keynote Speaker of the Kendric C. Smith Interdisciplinary Symposium in Photobiology, 38th American Society for Photobiology Meeting, Tampa, Florida (2016).
- 17) <u>2016 John S. Diekhoff Award for Distinguished Graduate Student Teaching</u>, Case Western Reserve University (2016).
- 18) Selected to participate in the <u>Denice D. Denton Emerging Leaders Workshop</u>, Madison, Wisconsin (2016).
- Guest Editor for a high profile Special Issue on "<u>Experimental and Computational Photochemistry of Bioorganic</u> <u>Molecules</u>" published in the journal <u>Molecules</u> as part of its 20th Anniversary (2016).
- 20) Invited lecture for The Power of Diversity Lectures Series. Office for Inclusion, Diversity and Equal Opportunity,

Case Western Reserve University (2015).

- 21) Selected in the 40-40 Club. Recognizes young Hispanic leaders in the Cleveland community (2010).
- 22) Frank Hovorka Assistant Professor of Chemistry, Case Western Reserve University (2012 2015).
- 23) Invited oral presentation as part of the *Diversity in Chemical Sciences* session presented at the 45<sup>th</sup> American Chemical Society Central Regional Meeting, Green Tree, Pittsburgh, PA; October 29 to November 1, 2014.
- 24) NSF Faculty CAREER Award, NSF Faculty Early Career Development Program (CAREER), National Science Foundation (2013 2018).
- 25) Carl Storm Underrepresented Minority Fellowship, to present a talk at the 2013 Gordon Research Conference on Photochemistry.

# PROFESSIONAL SERVICE

# Service to the University and Department

- Member of the Startup Success Committee, Case Western Reserve University, School of Medicine (2024 present).
- Member of the Postbaccalaureate Research Education Program (PREP) Steering Committee, Case Western Reserve University, School of Medicine (2023 – present).
- Dean's Liaison to the CAS Graduate Committee (2023 2023).
- Member of Case Western Reserve University Innovation Taskforce (2022 present).
- Member of Institute for Smart, Secure and Connected Systems Internal Advisory Board, Case Western Reserve University (2022 – present).
- Member of Case Western Reserve University Search Committee for Vice President for Research and Technology Management (2021 – 2022).
- Member of the President Commission on Student Success, Case Western Reserve University (2022 present).
- Member of Case Western Reserve University Northeast Ohio NMR Core Facility (2021 present).
- Member of Sears Think[box] Academics Research Committee, Case Western Reserve University (2022 present).
- Member of the College of Arts and Sciences Special Committee on Research (2022 present).
- Member of Case Western Reserve University Pathway 3 Industry Engagement and Innovation Advisory Committee (2021 – present).
- Member of the College of Arts and Sciences Executive Committee (2021 present).
- Member of Developmental Therapeutics Program, Case Comprehensive Cancer Center, CWRU School of Medicine (2020 – present).
- Member of the Steering Committee for Heart, Lung and Blood Summer Research Program, CWRU School of Medicine (2019 – present).
- Member and Mentor of the T32 Planning Committee for the Cleveland Center for Membrane and Structural Biology, CWRU School of Medicine (2020 present).
- Member of the 2021 Mentor Fellows Program, CWRU (2021 2022).
- Member of the College of Arts and Sciences Committee on Appointments (2020 2021).
- Member of the Shared Training to Advance Integrity in Research (STAIR) Mentor Fellows Program, CWRU (2019 2021).
- Faculty Advisor of the Chemistry Graduate Student Organization (2019 present).
- Member of the College of Arts & Science Graduate Committee (2018 2021).
- Member of the Chemistry Strategic Planning Committee (2018 2020).
- Member of the Graduate Affairs Committee (2017 present).
- Member of the Chemistry Graduate Admissions Committee (2017 present).
- Member of the NOA-AGEP Scholar Site Committee (2016 2012).
- Member of the President's Advisory Council on Minorities (2015 2022).
- Chair of the Faculty Search Committee (2018).
- Member of the Graduate Affairs Committee (2015 2016).
- Member of the Chemistry Resources Committee (2014 2017).

- Chair of the Chemistry Resources Committee (2014 2015).
- Annual recruiting travel to Puerto Rico to visit different campuses of the University of Puerto Rico system to promote CWRU and the Chemistry Department, to describe undergraduate summer research opportunities in our department, and to recruit underrepresented students into our graduate program (2012 present).
- Member of the College of Arts & Sciences Task Force on Research (2014 2016).
- Faculty Mentor of two Latino undergraduate students for the 'Más Allá de lo Posible' Mentoring Program at CWRU (2014 – 2015).
- Member of the Chemistry Visibility Committee (2011 2015).
- Chair and organizer of the Graduate Chemistry Retreat (2011 2013). In this event, 4th-year graduate students orally present their research work to the faculty and to other graduate students in the Department.
- Represented the Chemistry Department in the Annual Biomedical Research Conference for Minority Students (ABRCMS) on November 9 – 12 in St. Louis, MO, to promote the Department and to recruit underrepresented students to our graduate program (2011).
- Member of the Alpha Chi Sigma Chemistry Student Fraternity (2010 present).
- Program manager and coordinator of the ACS SEED Summer Program at CWRU: summer research experience for economically disadvantaged or underrepresented high school students in the Greater Cleveland area (2010 – present).
- Advisory Board Member of the Support of Undergraduate Research & Creative Endeavors at CWRU (2009
   – present).
- Member of the Energy and Material Science New Faculty Recruiting Committee (Spring 2008).
- Collaborated with Ms. Lisa Dunnigan, Assistant Director and Coordinator of Multicultural Student Recruitment Programs, Office of Undergraduate Admission, CWRU (2008 – 2011); participated in the Diversity Weekend Recruitment Brunch hosted by Undergraduate Admission.
- Member and advisor of the Graduate Minority Student Organization, School of Medicine, CWRU (2008 present).
- Reviewer for the CWRU Support of Undergraduate Research & Creative Endeavors (SOURCE) Program (2008 – present).
- Member of the Chemistry Executive Committee (2007 2008; 2013 2014; 2016).
- Collaboration with Ms. Churyl Croone, Assistant Director, International Student Recruitment Coordinator Territories: International Countries, to increase population of undergraduate students from Puerto Rico (2007–2013).
- Ongoing collaboration with Mr. Joseph T. Williams, Director, Office of Multicultural Programs (2007– present).
- Member of the Chemistry Graduate Admissions Committee (2007-2014).

# Workshops Organized

- Preparing and Delivering Scientific Talks (Fall 2011 & 2012). Given as part of the Graduate Chemistry Retreat. A workshop for 4th-year graduate students for preparing and delivering scientific talks and effective use of visual aids.
- Principles and Applications of Time-Resolved Spectroscopy: CERMACS09 Workshop and Open House hosted in the Center for Chemical Dynamics at Case Western Reserve University. A one-day workshop and hands-on experience for students, postdoctoral researchers, and faculty on principles and applications of time-resolved spectroscopy. Part of the CERMACS09 meeting. May 2009.
- Many Faces of STEM (Fall 2009). A workshop and hands-on experience for underrepresented 8<sup>th</sup> and 9<sup>th</sup> graders in the Cleveland Municipal School District focusing on science, technology, engineering, and mathematics (STEM) fields.
- Many Faces of STEM (Fall 2008). A workshop and hands-on experience for underrepresented 8<sup>th</sup> and 9<sup>th</sup> graders in the Cleveland Municipal School District focusing on science, technology, engineering, and mathematics (STEM) fields.

# Service to the Outside Scientific and Engineering Community

- Member of the Scientific Revision Board of the Puerto Rico Science, Technology and Research Trust (2022
   – present).
- Associate Editor of the Photochemistry and Photobiology journal (2021 present).
- Member of the Publications Committee for the American Society for Photobiology (2019 2022).
- American Society for Photobiology Engagement and Outreach Committee Member, Liaison for Latin America (2016 – present)
- Elected Member of the Council for the American Society for Photobiology (2016 2020)
- Chair of the American Chemical Society Canvassing Committee for the Ahmed Zewail Award in Ultrafast Science and Technology (2016 – 2019).
- Committee Member of Grants and Awards for the American Society for Photobiology (2011 2015).
- Active reviewer of peer-reviewed scientific journals. These include: Angewandte Chemie International Edition, Applied Physics Letters, Biochemistry, Chemical Communications, Chemical Physics Letters, ChemPhysChem, Chemical Sciences, Free Radical Biology & Medicine, International Reviews in Physical Chemistry, International Journal of Environmental Analytical Chemistry, Journal of Chemical Physics, Journal of Computational and Theoretical Chemistry, Journal of Molecular Structure, Journal of Photochemistry and Photobiology, Journal of Physical Chemistry A/B/C/Letters, Journal of the American Chemical Society, Langmuir, Molecules, Nature Chemistry, Nature Communications, Physical Chemistry Chemical Physics, Photochemistry and Photobiology, Photochemistry and Photobiology Sciences, Proceedings of the National Academy of Sciences, Radiation Research, and Spectrochimica Acta among others.
- Active ad hoc and panelist reviewer of proposals for the (1) National Science Foundation, including NSF-MRI, NSF-CRIF-MU, NSF-CMI, NSF-CSDM-A, NSF-GRFP, and NSF-FCAREER; (2) ACS Petroleum Research Fund; (3) Swiss National Science Foundation; (4) U. S. Department of Energy, Office of Science; (5) Research Corporation for Science Advancement (Cottrell College Science Award); (6) the Ohio Supercomputer Center; and (7) Puerto Rico Science, Technology and Research Trust.
- Member of the 2020 Committees of Visitors (COVs) at NSF. COVs are subcommittees of NSF directorate
  advisory committees and provide NSF with external expert assessments of the quality and integrity of
  program operations, program management, and the breadth of program portfolios.

# **Conferences Organized**

- Symposium Chair: XVI ELAFOT / 2<sup>nd</sup> LatASP Meeting, Panamá City, Panamá. Symposium: Photodynamic Therapy and Photodynamic Inactivation. October 27 to 30, 2025.
- Symposium Chair: The 42<sup>nd</sup> Biennial Meeting of the American Society for Photobiology, Chicago, Illinois, July 27 to 30, 2024.
- Symposium Chair: The 41<sup>st</sup> Biennial Meeting of the American Society for Photobiology, Albuquerque Hotel, Albuquerque, New Mexico. September 25-28, 2022.
- Symposium Chair: The 40<sup>th</sup> Biennial Meeting of the American Society for Photobiology, Sheraton Grand Chicago, Chicago, Illinois. June 27-30, 2020. (This meeting was moved online because of the COVID-19 pandemic).
- Symposium Chair: The 39<sup>th</sup> Biennial Meeting of the American Society for Photobiology, Tampa Bay, Florida. Symposium: Direct and Sensitized Photochemistry in Biological Molecules (two sessions). May 12-15, 2018.
- Symposium Chair: The 38<sup>th</sup> Biennial Meeting of the American Society for Photobiology Meeting, Tampa, Florida. Symposium: Current Topics in Photobiology, II. May 21-26, 2016.
- Organizer: The Seventy-Third Frontiers in Chemistry Series on Biophotonics, Case Western Reserve University, Department of Chemistry, Spring 2014.
- Symposium Chair: Astrobiology Science Conference 2012, Atlanta, Georgia, April 16-20, 2012.
- Chair of the Physical Chemistry General Sessions: 2009 Central Regional Meeting of the American Chemical Society (CERMACS09). May 20-23, 2009.
- Symposium Chair: The 33<sup>rd</sup> Biennial Meeting of the American Society for Photobiology Meeting, Río Grande, Puerto Rico. Symposium: Early Events in Photochemistry and Photobiology: Session I. Ultrafast

Excited State Dynamics and Charge Transfer in DNA and Session II. Fast Processes in DNA Photorepair, DNA Interactions, and Proteins. July 2006.

## **REVIEWED BOOKS**

• Oliver Schalk and Enrico Tapavicza, *Photochemistry*, American Chemical Society's ACS In Focus series, American Chemical Society Publications, March 2021, <u>DOI:10.1021/acs.infocus.7e4009</u>.

# **TEACHING / MENTORING**

**Courses Taught** 

- CHEM 451/351: Bioorganic and Environmental Photochemistry, Spring 2024, 3 credit hours.
- CHEM 506: Bioorganic and Environmental Photochemistry, Fall 2019, 3 credit hours.
- CHEM 447: Modern Physical Chemistry (team-teach), Fall 2019 & 2022, 3 credit hours.
- CHEM 332: Laboratory Methods in Physical Chemistry, Spring 2008, 2009, 2010, 2011, 2017, 2018, 2019, 2020, 2021, 2022 & 2023, 3 credit hours.
- CHEM 305: Introduction to Laboratory Methods in Physical Chemistry, Spring 2009, 2010, 2011, 2017,2018, 2019, 2020, 2021, 2022, & 2023, 3 credit hours.
- CHEM 446/337: Quantum Mechanics I, Fall 2008, 2010, 2012, 2015, & 2017 3 credit hours.
- CHEM 406: Chemical Kinetics, Fall 2009, 2011, 2014, 2016, 2018, & 2020 3 credit hours.
- CHEM 336: Physical Chemistry II, Spring 2012, 2013, 2014, 2015, & 2016, 3 credit hours.

# Visiting Researcher (Sabbatical)

1) Assoc. Prof. Karl Feierabend (07/01/2018 – 06/30/2019; The College of Wooster, Wooster, OH)

## Post Graduate Associates

- 1) Dr. Amy Sage (02/01/2008 11/30/2008).
- 2) Dr. Christian Reichardt (04/01/2008 02/28/2011)
- 3) Dr. Olexandr Isayev (04/01/2009 02/01/2012)
- 4) Dr. Matthew Brister (06/01/2018 07/31/2018)
- 5) Dr. Sourav K. Seth (12/01/2021 present)
- 6) Dr. Reshma Mathew (03/28/2024 present)

# **Graduate Students**

1) R. Aaron Vogt (start date 01/08/2007, Ph.D. completed 12/2012)

- 2) Chengwei Wen (start date 01/08/2008; Master completed on 12/2011)
- 3) Cao Guo (start date 01/08/2009; Master completed on 12/2011)
- 4) Qing Wang (start date 01/08/2009; Master completed on 12/2011)
- 5) Huijuan Huang (start date 01/08/2010; Master completed on 07/2013)
- 6) Nicholas Dunn (start date 01/08/2011; Master completed on 06/2015)
- 7) Hikari Katadai (start date 10/01/2015; Master completed on 05/2016)
- 8) Marvin Pollum (start date 01/08/2011; Ph.D. completed 12/2016)
- 9) Matthew Brister (start date 01/11/2012; Ph.D. completed 5/2018)
- 10) Regina DiScipio (start date 01/11/2013; Ph.D. completed 5/2018)
- 11) Glesmarie Ortíz-Zayas (Master completed on 05/2019)
- 12) Luis Ortiz-Rodríguez (start date 01/11/2017; Ph.D. completed on 5/2022)
- 13) Naishka Caldero Rodríguez (start date 01/11/2017; Ph.D. completed on 5/2022)
- 14) Sean J. Hoehn (start date 01/11/2017; Ph.D. completed on 6/2022)
- 15) Cameron Griffith (start date 01/12/2018; Ph.D. completed on 7/2023)
- 16) Sarah Krul (start date 14/06/2019; Ph.D. completed on 5/2022)
- 17) Ergian Mao (start date 08/1/2021; Master completed 05/2022)
- 18) Chris Acquah (start date 01/21/2020; ongoing Ph.D.)
- 19) Rubej Khan (start date 11/1/2022; ongoing Ph.D.)

20) Karitza Díaz-González (start date 11/1/2022; NSF-GRFP honorary mention; ongoing Ph.D.)

21) Nitza V. Falcón-Cruz (start date 12/8/2023; NSF-GRFP fellow; ongoing Ph.D.)

22) Tazrin Islam Tonny (start date 12/8/2023; ongoing Ph.D.)

23) Kushan Thanthiriwaththage-Don (start date 12/2/2024; ongoing Ph.D.)

## **Undergraduate Students**

1) Jeff Lyvers (2008) Department of Pharmacology, Case Western School of Medicine.

2) Bradley Sutton (2008 – 2009) Epic Systems Corporation in Madison, WI.

3) Do-Yong Kim (2008 – 2009) Graduate student at Texas A&M University, Department of Chemistry.

4) Joyann Marks (Fisk University, summer 2009) ACES NSF-Advance 2009 Summer Research Program Fellow.

5) Leah Dodson (2008 – 2010) Graduate student at California Institute of Technology, Department of Chemistry. Currently, Assistant Professor, Department of Chemistry and Biochemistry, University of Maryland, College Park, MD.

6) Saeed Rahman (2008 – 2010) Graduate student at Columbia University.

7) Ricardo Vidot (2008 – 2011) ACS Scholars Fellow.

8) Veronica Laos (2011 – 2014) Graduate student at University of California at Santa Barbara, Department of Chemistry.

9) Hannah Jenkins (2011 – 2015)

10) Akash Adhia (2012 – 2014) Feinberg School of Medicine, Northwestern University.

11) Kelsie Leary (2013 – 2015) Graduate student at Dartmouth College, Department of Chemistry.

12) Margaret Angus (2014 – 2015)

13) John Landschulz (2014 – 2015)

14) Andrew López (start date 01/11/2014 – 2015; as part of 'Más Allá de lo Posible' Mentoring Program)

15) Dhariyat Menendez (start date 01/11/2014 – 2015; as part of '*Más Allá de lo Posible*' Mentoring Program)

16) Brennan Ashwood (2014 – 2017) Graduate student at University of Chicago, Department of Chemistry.

17) Eric Jiang (2015 – 2016; 2018)

18) Kieran Farrell (2016 – 2018) Graduate student at University of Wisconsin-Madison.

19) Raymond Santiago (REU, summer 2016)

20) Luis Ortiz-Rodríguez (University of Puerto Rico, Humacao Campus, REU, summer 2014, 2015 & 2016)

21) Michael Ward (summer 2016)

22) Kathleen H. Tong (summer 2017)

- 23) Anna Goff (2018)
- 24) Howard (Bradley) Walker (2018 2019)

25) Lidia Waidmann (2018 – 2020)

- 26) Collin Merrick (2018 2021)
- 27) Andres Gonzalez (2019 2021)
- 28) Benjamin Klucznik (2019 2022)
- 29) Mia Formato (2019 2021)
- 30) Nadia Abbass (2019 2021)
- 31) BrandonJ. Skory (2020 2022)
- 32) Adina Minkin (2020 2021)
- 33) Grace Sleyko (2021 2022)
- 34) Onel O. Ortiz-Esteves (2021 2022)
- 35) Michael Pogharian (2020 2023)
- 36) Kevin Van Allen (2021 2022)
- 37) Tram Phan (2021 2022)
- 38) Eric Lee (2022 present)
- 39) Daniella Fish (2022 2023)
- 40) Medha Patria (2022 2023)
- 41) Salman Elahi (2022 2023)
- 42) Sabrina Soto (2023 2024)

43) Arjun Saulnier (2024 - present)

44) Capri Reyes (2024 – present)

# **High School Students**

- 1) Courtney Johnson (summer 2008)
- 2) Matthew Beard (summer 2010; ACS-SEED Program)
- 3) Briana Sealey (summer 2011 & summer 2012; ACS-SEED Program)
- 4) Omar Mahmoud (summer 2012; ACS-SEED Program)
- 5) Raymond Santiago (summer 2013 & 2014; ACS-SEED Program)
- 6) Jessica Pham (summer 2014; ACS-SEED Program)
- 7) Erica Truong (summer 2014 & 2015; ACS-SEED Program)
- 8) Frankie Santiago (summer 2015 & 2016; ACS-SEED Program)
- 9) Daisha Taylor (summer 2016 & 2017; ACS-SEED Program)
- 10) Dawn Luong (summer 2017 & 2018; ACS-SEED Program)
- 11) Monai Wilson (summer 2018; ACS-SEED Program)
- 12) Rayele Malone (summer 2018 & 2019; ACS-SEED Program)
- 13) Dharma Hutson (summer 2022; summer 2023)
- 14) Ashley Feliciano (summer 2023; ACS-SEED Program)
- 15) Kamila Maldonado (summer 2024 & 2025; ACS-SEED Program)
- 16) Anna Johannessen (summer 2024; Gilmour Academy, Catalyst Program)

## **Visiting Students**

1) Joyann Marks (Undergraduate Student, Fisk University, summer 2009). ACES NSF-Advance 2009 Summer Research Program Fellow.

2) María Morel (Graduate Student, University of Puerto Rico, San Juan Campus, 2009).

- 3) Lara Martínez (Graduate Student, Universidad Autónoma de Madrid, Madrid, Spain, 02/2013 04/2013)
- 4) Luis Ortiz-Rodríguez (University of Puerto Rico, Humacao Campus, summer 2014, 2015 & 2016)
- 5) Serra Arskancan (Graduate Student, Universidad Autónoma de Madrid, Madrid, Spain, 05/2016 08/2016)

6) Ana Belén Fraga Timiraos (Graduate Student, Universitat Politècnica de València, València, Spain, 09/2016 – 12/2016)

7) Enrique Arpa (Graduate Student, Universidad Autónoma de Madrid, Madrid, Spain, 03/2018 – 07/2018)

8) Brandon J. Skory (Baldwin Wallace University, Berea, Ohio)

9) Onel O. Ortiz-Esteves (Undergraduate Student, University of Puerto Rico, Mayaguez Campus, 2022)

10) Isaiah Gilbert (Undergraduate Student, Northwestern University, Evanston, IL, INSPIRE-US Summer Research Program 2025)

# **Recent Synergistic Activities**

# Broadening the participation of underrepresented groups in science, mathematics, engineering and technology

- Program manager and coordinator of the ACS SEED Summer Program at CWRU (2010 present). Summer research experience for economically disadvantaged or underrepresented high school students in Cleveland.
- Advisory Board Member of the Support of Undergraduate Research & Creative Endeavors at CWRU (2009 2021).
- Research mentor of high-school students on the Mentor Matching Engine, an invitation-based platform to bring together mentors, students and teachers who can collaborate on student research projects in science, technology, engineering, and mathematics (STEM) fields. The Mentor Matching Engine is a central feature of the R&D STEM Learning Exchange's offerings as part of the Illinois Pathways Initiative (2019 – 2020).
- Associated Faculty of the Minority Graduate Student Organization (MGSO) at Case Western Reserve University (2007 – present). The MGSO was formed in 2001 to foster a student group identity and shared values. The MGSO meets once a month to discuss members' research experiences.

- Reviewer for the CWRU Support of Undergraduate Research & Creative Endeavors (SOURCE) Program (2008 – 2021).
- Faculty mentor of two Latino undergraduate students (Ms. Dhariyat Menendez and Mr. Andrew Lopez) for the "Más Allá de lo Posible" mentoring program at CWRU (2014 2015).
- Many Faces of STEM, 2008 2011. I was actively involved in workshops for underrepresented 8<sup>th</sup> and 9<sup>th</sup> graders in the Cleveland Municipal School District focusing on science, technology, engineering, and mathematics (STEM) fields. The primary goal was to strengthen STEM concepts and motivate students to follow STEM career path in the future. This was a joint effort with Dr. LaShanda Korley, African American and Assistant Professor of Macromolecular Science and Engineering Department at Case Western Reserve University.
- ACS-Scholars Mentoring Consultant (2007 2012). I was university mentor of Mr. Ricardo Vidot, who is member of an underrepresented minority group in the Department of Chemistry at CWRU.

# ADMINISTRATION / ASSOCIATE DEAN FOR RESEARCH PORFOLIO (July 2021 - present)

Reporting to the Dean, the Associate Dean for Research (ADR) is a member of the leadership team in the College Dean's Office and works closely with the school's other Associate Deans and department chairs and staff to seek excellence in the College. The ADR is responsible for leading efforts to advance and support research, scholarship, and creative works across the College. **This is an administrative position with 50% effort as Associate Dean in College administration and 50% effort in the tenured faculty position**. This position serves at the pleasure of the dean.

### Key Responsibilities and Duties (in no particular order)

1. Lead efforts to advance research, scholarly works, and creative endeavors across the 21 Departments of the College

2. Facilitate the advancement of research, scholarly works and creative endeavors and the increase of external funding from federal agencies, foundations, and industry (responsible for stimulating new and continued research activity)

3. Benchmark departments and faculty performance in research relative to peer institutions

4. Oversee CAS research administration, compliance, and grant matches, including supervising the Assistant Dean of Research Administration who leads the CAS Office of Research

5. Foster a collaborative and interdisciplinary environment for research across departments, centers, and the University

6. Serve as the CAS liaison to the University's Office of Research and Technology Management and the SPARC Team

7. Liaison with the Office of Strategic Giving, the Office of Foundation Relations, the Office of Corporate Relations, and the Office of Government and Community Relations for proposal development and reporting

8. Oversee and coordinate needs for equipment for research; assist with start-up packages for new faculty hires

- 9. Enhance research support for graduate students and post-docs (with AD for Academic Affairs)
- 10. Oversee the Expanding Horizons Initiative in conjunction with the Assistant Dean of Research

11. Oversee Effort Reporting and Conflict of Interest policies in research

12. Assist the dean and other university administrators with faculty misconduct related to research

13. Serve as the CAS liaison to the institutional core facilities committee

14. Lead programming efforts to enhance research mentoring and identification of funding sources, career development, and grant writing workshops

15. Review/approve Institutional Review Board (IRB) applications submitted by department chairs for research projects

16. Work with the dean to create equity in resource support for research/scholarship across the sciences, arts and humanities

17. Work with the dean to implement the university & college's strategic plans in all relevant areas

18. Review and approve proposals for the W.P. Jones Presidential Faculty Development Program, EHI-Finish

Line Funds, EHI-Pre Review Fund, EHI-Social and Racial Justice Grants, EHI-Teaching Innovation Grant, and the Morrell Heald Endowed Fund for Curricular Innovation

19. Evaluate and rank university-wide proposals with limited institutional submissions (together with other ADRs), including for the Camille Dreyfus Teacher-Scholar Awards, Blavatnik National Laureate Award for Young Investigator, NSF MRI Track 2 Applications, NSF MRI Internal Submission, CWRU-Faculty Distinguished Research Award, Searle Candidate Selection Awards, among others

20. Help coordinate interdisciplinary, multi-principal investigator research proposals, research center proposals and training grants

21. Ensures that the college follows best practices in the management and oversight of funded research initiatives, scholarly works, and creative endeavors

22. Review/approve the Proposal Initiation Forms (PIF) requesting course releases, course by-outs, sabbaticals, changes in the negotiated F&A, use of off-campus F&A, and foundation/industry proposals that do not allow F&A or allow as significantly lower F&A

23. Review and approve annual research spending, funding trends, and research productivity reports, CAS Newsletters, etc. generated by the CAS Research Office for the Provost, CAS Dean, and VP for Research, CAS Visiting Committee

24. Travel/visit/assist the VP for Research to created partnerships with industry and national labs including NASA Glen Research Center, the Air Force Research Laboratory (Wright-Patterson AFB and Wright Brothers Institute), Intel, StarLab, Lubrizol, ULRI, among others

25. Assist/review in space planning (CAS & ISEB) with Associate Dean for Strategic Initiatives, Finance and Administration and Director of Facilities Management

26. Review and provide recommendations of departmental external reviews

27. Meet with candidates for tenure-track and non-tenure-track faculty hire positions

28. CAS representative as a member of the Smart, Secure and Connected Systems Internal Advisory Board, Startup Success Committee, CWRU Innovation Taskforce, President Commission on Student Success, Northeast Ohio NRM Core Facility, Sears Think[box] Academics Research Committee, CWRU Pathway 3 Industry Engagement and Innovation Advisory Committee

### Primary Academic and Administrative Achievements Since 2019

Dr. Carlos E. Crespo-Hernández is a leading figure in the field of photochemistry and photobiology, recognized for his research breakthroughs and dedication to nurturing aspiring scientists. He is currently a Professor and Associate Dean for Research in the College of Arts and Sciences at Case Western Reserve University (CWRU). He has more than 20 years of research and training experience working at R1 institutions in the USA. Dr. Crespo has a track record of external funding from federal agencies and national foundations, and his research group has been continuously funded since 2008. He has demonstrated a record of scholarly achievement appropriate for a senior career level, with one patent, two invention disclosures, +120 peer-reviewed papers, 4 book chapters, and 7 review articles, including 6 publications in flagship journals such as Nature (3), Science (1), Nature Commun. (2), and PNAS (2), and +\$3M in major extramurally funded research grants as a principal investigator; the ability to collaborate across disciplines; and a positive and supportive team spirit. Dr. Crespo-Hernández research in biophysical, computational, organic, and physical chemistry, with application in the photodynamic therapy of cancers and cell bioimaging, is multidisciplinary, interdisciplinary, and highly collaborative. He has chaired or co-chaired 11 national and international research conference symposia, give +100 invited talks, and published +160 research abstracts. Dr. Crespo-Hernández has demonstrated the ability to build national and international collaborations and coordinate initiatives among faculty, academic, administrative, and community constituents. During his entire career, Dr. Crespo-Hernández has established trusting partnerships and relationships with many prominent academic scientists in Argentina, Austria, Brazil, China, Denmark, France, Japan, Italy, Spain, Ukraine, and the USA, and he is determined to work with groups and individuals who are also trying to address the complex research challenges that confront us today. Dr. Crespo-Hernández is a scientist who is a nationally and internationally recognized scholar and whose accomplishments reflect sustained research excellence in the chemistry field and higher education.

Dr. Crespo-Hernández has demonstrated leadership, management, and administrative experience, including managing and coordinating the American Chemical Society SEED Summer Program at CWRU since 2010, codirecting the Center for Chemical Dynamics from 2008 to 2018, advocating and playing a key role in the establishment of a newly formed Ultrafast Laser Facility in the Department of Chemistry, managing federal (NSF and DoD) and foundation (ACS-PRF) budgets, and supervising high school (25), undergraduate (63), and graduate students (28), and 6 postdoctoral fellows (+120 total since 2007). He has management and administrative experience leading a research team and collaborators since 2007, managing projects and budgets, supervising students, and postdoctoral fellows, evaluating research activities and initiatives, and achieving short and long-term goals. Since 2021, Dr. Crespo-Hernández has been appointed Associate Dean for Research in the College of Arts and Sciences at CWRU, where he manages a ca. \$40M research portfolio and serve 300 faculty members. He is an appointed member of the American Chemical Society Board Standing Committee on the Petroleum Research Fund, the Scientific Revision Board of the Puerto Rico Science, Technology and Research Trust, and of the Institute for Smart, Secure and Connected Systems Internal Advisory Board, Case Western Reserve University. Dr. Crespo-Hernández has also demonstrated success leading research initiatives and a track record of open, transparent communications, proactively building positive relationships with faculty, staff, students, and diverse constituents. He has demonstrated commitment to equal opportunity for all, and the ability to manage sensitive and confidential information. Dr. Crespo-Hernández is a Faculty Co-Advisor of the Chemistry Graduate Student Organization, a member of the Graduate Minority Organization, and have served for more than ten years as a member of the Graduate Admission Committee in the Department of Chemistry. He is also an advisory board member of the Support of Undergraduate Research & Creative Endeavors; member of the Alpha Chi Sigma Chemistry Student Fraternity; member of the NOA-AGEP Scholar Site Committee; member of the Steering Committee of Heart, Lung and Blood Summer Research Program, CWRU School of Medicine; member and mentor of the T32 planning committee for Cleveland Center for Membrane and Structural Biology, CWRU School of Medicine. In 2020, he was selected as a STAIR Mentor Fellow to enhance his mentoring relationship with a junior faculty member in our department, and he was selected as a member of the Mentor Fellows Program in 2021. These and many other activities have provided him with the necessary experience in mentoring junior faculty, researchers, postdoctoral scholars, and students, working with multicultural populations, and promoting excellence in education, research, and administration. Since Dr. Crespo-Hernández hit the ground running at CWRU, he has been committed to empowering innovative research, scholarship, and creative activities that drive knowledge creation and technological innovations, focused on improving society.

### Major research accomplishments and contributions

- Research in photochemistry and photobiology: Crespo-Hernández's research focuses on light-induced phenomena in molecules, biopolymers, and cells. His work aims to understand the mechanistic aspects of these processes at the molecular level, particularly their relevance to cancer therapy, renewable energy, and the environment.
- 2. Ultrafast electronic spectroscopy and chemical dynamics: A key aspect of his research involves using ultrafast electronic spectroscopy to study excited-state dynamics in molecules. This includes investigating how molecules in human cells, or prescribed as medicines, can trigger damage to cellular DNA when exposed to sunlight. His work also explores the use of his discoveries in developing safer drugs and new anticancer agents.
- 3. DNA photostability, photodamage, and intersystem crossing dynamics: His research has delved into understanding how UV radiation affects DNA and the photochemistry of DNA/RNA nucleobases and their derivatives. He has investigated the electronic deactivation mechanisms that give rise to the efficient population of long-lived and reactive triplet states, a key aspect of intersystem crossing dynamics in these

molecules. His work has shown that sulfur-substituted nucleobases (thiobases) can have significantly redshifted absorption spectra compared to their natural counterparts. Excitation of these thiobases with near-visible light leads to ultrafast population of the triplet state, with some exhibiting remarkably short intersystem crossing lifetimes of ca. 100 fs and high singlet oxygen quantum yields, making them potent photosensitizers.

4. Heavy-atom-free photosensitizers: Crespo-Hernández has made significant contributions to developing novel applications such as photomedicines, including the design and investigation of heavy-atom-free photosensitizers for photodynamic therapy. Recently, his work in this area led to the development of 5-(5phenylthiophen-2-yl)-6-azauridine, a three-pronged agent for cell imaging, cancer cell inhibition and a promising candidate for PDT applications.

In summary, Carlos E. Crespo-Hernández is a recognized leader. His contributions encompass a wide range of topics in physical chemistry, computational chemistry, and photochemistry, from fundamental investigations into DNA photodamage and intersystem crossing dynamics to developing new photomedicines and photosensitizers for cancer treatment. His commitment to both research and education has made him a respected figure in the scientific community.

### RESEARCH / SCHOLARSHIP Proposal and Award Activity Current and Completed Proposals

- 2025 ACS SEED Summer Program at CWRU; PI: Crespo; Source of Support: ACS; Total Award Amount: \$22,000; Total Direct Costs: \$13,600; Percent Effort: 2%; Total Award Period Covered: 7/2025–6/2026; Support: current.
- 2024 ACS SEED Summer Program at CWRU; PI: Crespo; Source of Support: ACS; Total Award Amount: \$24,000; Total Direct Costs: \$15,600; Percent Effort: 2%; Total Award Period Covered: 7/2024–6/2025; Support: completed.
- Prebiotic Chemistry and the Molecular Origins of Life; PI: Crespo; Source of Support: EHI (CAS/CWRU); Total Award Amount: \$18,000.00; Total Direct Costs: \$ 18,000.00; Percent Effort: 2%; Total Award Period Covered: 5/2024–4/2025; Support: current.
- 4) Development of Photosensitizers for the Treatment of Cancer Cells Absorbing Two Photons in the Near Infrared, PI: Crespo; Source of Support: EHI-CAS; Total Award Amount: \$36,350; Total Direct Costs: \$36,350; Percent Effort: 2%; Total Award Period Covered: 5/2023–4/2024; Support: current.
- 5) ACES+ Grant: Development of Light-Activated Therapy Agents Absorbing in the Near Infrared for the Treatment of Cancer Cells, PI: Crespo; Source of Support: ACSE+/CWRU; Total Award Amount: \$5,000; Total Direct Costs: \$5,000; Percent Effort: 0.1%; Total Award Period Covered: 5/2023–4/2024; Support: completed.
- 6) Deliberate Design and Synthesis of Thionated Organic Photosensitizers Activated by One- and Two-Photon Absorption in the Near-Infrared; PI: Crespo; Source of Support: NSF; Total Award Amount: \$535,000.00; Total Direct Costs: \$ 347,634.00; Percent Effort: 10%; Total Award Period Covered: 7/2023– 6/2026; Support: current.
- 7) Structure-Photoreactivity Relationships in Polycyclic Aromatic Sulfur Heterocycle Pollutants; PI: Crespo; Source of Support: ACS-PRF; Total Award Amount: \$110,000; Total Direct Costs: \$110,000; Percent Effort: 2%;

Total Award Period Covered: 9/2022–8/2024; Support: completed.

- 2023 ACS SEED Summer Program at CWRU; PI: Crespo; Source of Support: ACS; Total Award Amount: \$16,000; Total Direct Costs: \$15,200; Percent Effort: 2%; Total Award Period Covered: 6/2023–6/2024; Support: completed.
- 9) Supplementary Funds, Instrument." (Electronic Relaxation Pathways in Nucleic Acid Derivatives Based on Functionalization of the Pyrimidine Chromophore; CHE-1800052); PI: Crespo; Source of Support: NSF; Total Award Amount: \$28,000.00; Total Direct Costs: \$ 59,018.00; Percent Effort: 1%; Total Award Period Covered: 7/2021–6/2022; Support: completed.
- 2022 ACS SEED Summer Program at CWRU; PI: Crespo; Source of Support: ACS; Total Award Amount: \$3,200; Total Direct Costs: \$2,700; Percent Effort: 2%; Total Award Period Covered: 6/2022–6/2023; Support: completed.
- 11) Supplementary Funds, Mitigation of COVID-19 Impact Supplementary Funds." (Electronic Relaxation Pathways in Nucleic Acid Derivatives Based on Functionalization of the Pyrimidine Chromophore; CHE-1800052); PI: Crespo; Source of Support: NSF; Total Award Amount: \$90,000.00; Total Direct Costs: \$ 59,018.00; Percent Effort: 1%; Total Award Period Covered: 7/2021–6/2022; Support: completed.
- 12) Supplementary Funds, MPS Alliances for Graduate Education and the Professoriate Graduate Research Supplements (AGEP-GRS)." (Electronic Relaxation Pathways in Nucleic Acid Derivatives Based on Functionalization of the Pyrimidine Chromophore; CHE-1800052); PI: Crespo; Source of Support: NSF/AGEP-GRS; Total Award Amount: \$61,443.00; Total Direct Costs: \$44,973.00; Percent Effort: 1%; Total Award Period Covered: 1/2021–6/2022; Support: completed.
- 13) International Supplementary Funds (Electronic Relaxation Pathways in Nucleic Acid Derivatives Based on Functionalization of the Pyrimidine Chromophore; CHE-1800052); PI: Crespo; Source of Support: NSF; Total Award Amount: \$17,728; Total Direct Costs: \$10,600; Percent Effort: 1%; Total Award Period Covered: 7/2019–6/2022; Support: completed.
- 14) Electronic Relaxation Pathways in Nucleic Acid Derivatives Based on Functionalization of the Pyrimidine Chromophore (CHE-1800052); PI: Crespo; Source of Support: NSF; Total Award Amount: \$450,000; Total Direct Costs: \$306,932; Percent Effort: 10%; Total Award Period Covered: 7/2018–6/2022; Support: completed.
- 2020 ACS SEED Summer 1 Program at CWRU; PI: Crespo; Source of Support: ACS; Total Award Amount: \$24,500; Total Direct Costs: \$19,600; Percent Effort: 2%; Total Award Period Covered: 6/2020–6/2021; Support: canceled because of COVID-19.
- 16) 2020 ACS SEED Summer 2 Program at CWRU; PI: Crespo; Source of Support: ACS; Total Award Amount: \$4,100; Total Direct Costs: \$3,300; Percent Effort: 2%; Total Award Period Covered: 6/2020–6/2021; Support: canceled because of COVID-19.
- 2019 ACS SEED Summer 1 Program at CWRU; PI: Crespo; Source of Support: ACS; Total Award Amount: \$10,000; Total Direct Costs: \$9,400; Percent Effort: 2%; Total Award Period Covered: 6/2019–6/2020; Support: completed.
- 2019 ACS SEED Summer 2 Program at CWRU; PI: Crespo; Source of Support: ACS; Total Award Amount: \$12,000; Total Direct Costs: \$11,200; Percent Effort: 2%; Total Award Period Covered: 6/2019–6/2020; Support: completed.

- 2018 ACS SEED Summer 1 Program at CWRU; PI: Crespo; Source of Support: ACS; Total Award Amount: \$10,000; Total Direct Costs: \$9,400; Percent Effort: 2%; Total Award Period Covered: 6/2018–6/2019; Support: completed.
- 20) 2018 ACS SEED Summer 2 Program at CWRU; PI: Crespo; Source of Support: ACS; Total Award Amount: \$9,000; Total Direct Costs: \$8,400; Percent Effort: 2%; Total Award Period Covered: 6/2018–6/2019; Support: completed.
- 21) International Supplementary Funds (NSF Faculty CAREER: Mechanistic Investigations of the Excited-State Dynamics in Thiobase and Pterin UVA Sensitizers and in Their DNA Constructs; CHE-1641304); PI: Crespo; Source of Support: NSF; Total Award Amount: \$16,642; Total Direct Costs: \$10,600; Percent Effort: 1%; Total Award Period Covered: 6/2016–9/2018; Support: completed.
- 22) Research Experience for Undergraduates (Supplementary Funds to NSF Faculty CAREER: Mechanistic Investigations of the Excited-State Dynamics in Thiobase and Pterin UVA Sensitizers and in Their DNA Constructs; CHE-1539808); PI: Crespo; Source of Support: NSF; Total Award Amount: \$5,748; Percent Effort: 1%; Total Award Period Covered: 6/2015–9/2018; Support: completed.
- 23) NSF Faculty CAREER: Mechanistic Investigations of the Excited-State Dynamics in Thiobase and Pterin UVA Sensitizers and in Their DNA Constructs (CHE-1255084); PI: Crespo; Source of Support: NSF CAREER; Total Award Amount: \$584,200; Total Direct Costs: \$400,736; Percent Effort: 10%; Total Award Period Covered: 4/2013–9/2018; Support: completed.
- 24) 2017 ACS SEED Summer 1 Program at CWRU; PI: Crespo; Source of Support: ACS; Total Award Amount: \$9,000; Total Direct Costs: \$7,500; Percent Effort: 2%; Total Award Period Covered: 6/2017–6/2018; Support: completed.
- 25) 2017 ACS SEED Summer 2 Program at CWRU; PI: Crespo; Source of Support: ACS; Total Award Amount: \$31,500; Total Direct Costs: \$30,000; Percent Effort: 2%; Total Award Period Covered: 6/2017–6/2018; Support: completed.
- 26) 2016 ACS SEED Summer 1 Program at CWRU; PI: Crespo; Source of Support: ACS; Total Award Amount: \$30,500; Total Direct Costs: \$30,500; Percent Effort: 2%; Total Award Period Covered: 6/2016–6/2017; Support: completed.
- 27) 2016 ACS SEED Summer 2 Program at CWRU; PI: Crespo; Source of Support: ACS; Total Award Amount: \$3,000; Total Direct Costs: \$3,000; Percent Effort: 2%; Total Award Period Covered: 6/2016–6/2017; Support: completed.
- 28) 2015 ACS SEED Summer 1 Program at CWRU; PI: Crespo; Source of Support: ACS; Total Award Amount: \$17,500; Total Direct Costs: \$14,500; Percent Effort: 2%; Total Award Period Covered: 7/2015–6/2016; Support: completed.
- 29) 2015 ACS SEED Summer 2 Program at CWRU; PI: Crespo; Source of Support: ACS; Total Award Amount: \$12,000; Total Direct Costs: \$12,000; Percent Effort: 2%; Total Award Period Covered: 7/2015–6/2016; Support: completed.
- 2014 ACS SEED Summer 1 Program at CWRU; PI: Crespo; Source of Support: ACS; Total Award Amount: \$14,500; Total Direct Costs: \$14,500; Percent Effort: 2%; Total Award Period Covered: 7/2014–6/2015; Support: completed.

- 2014 ACS SEED Summer 2 Program at CWRU; PI: Crespo; Source of Support: ACS; Total Award Amount: \$13,600; Total Direct Costs: \$13,600; Percent Effort: 2%; Total Award Period Covered: 7/2014–6/2015; Support: completed.
- 32) **2013 ACS SEED Summer 1 Program at CWRU**; PI: Crespo; Source of Support: ACS; Total Award Amount: \$10,000; Total Direct Costs: \$10,000; Percent Effort: 2%; Total Award Period Covered: 7/2013–6/2014; Support: completed.
- 33) 2013 ACS SEED Summer 2 Program at CWRU; PI: Crespo; Source of Support: ACS; Total Award Amount: \$6,000; Total Direct Costs: \$6,000; Percent Effort: 2%; Total Award Period Covered: 7/2013–6/2014; Support: completed.
- 34) 2012 ACS SEED Summer 1 Program at CWRU; PI: Crespo; Source of Support: ACS; Total Award Amount: \$6,400; Total Direct Costs: \$6,400; Percent Effort: 2%; Total Award Period Covered: 7/2012–6/2013; Support: completed.
- 35) 2012 ACS SEED Summer 2 Program at CWRU; PI: Crespo; Source of Support: ACS; Total Award Amount: \$7,400; Total Direct Costs: \$7,400; Percent Effort: 2%; Total Award Period Covered: 7/2012–6/2013; Support: completed.
- 36) **2011 ACS SEED Program at CWRU**; PI: Crespo; Source of Support: ACS; Total Award Amount: \$9,600; Total Direct Costs: \$9,600; Percent Effort: 2%; Total Award Period Covered: 7/2011–6/2012; Support: **completed**.
- 37) Binding of DNA Components to Nitro-Compounds (Renewal; DoD-W912HZ-11-1-0003); PI: Crespo; Source of Support: DoD/USACE-Army Corps of Engineers; Total Award Amount: \$53,501; Total Direct Costs: \$39,630; Percent Effort: 5%; Total Award Period Covered: 1/2011–1/2012; Support: completed.
- 38) Photochemistry of Environmentally Relevant Nitro-Polycyclic Aromatic Hydrocarbons (ACS-PRF-48755-DNI4); PI: Crespo; Source of Support: ACS-PRF; Total Award Amount: \$100,000; Total Direct Costs: \$100,000; Percent Effort: 2%; Total Award Period Covered: 1/2009–8/2011; Support: completed.
- 39) Binding of DNA Components to Nitro-Compounds (Renewal; DoD-W912HZ-09-C-0028); PI: Crespo; Source of Support: DoD/USACE-Army Corps of Engineers; Total Award Amount: \$127,956; Total Direct Costs: \$94,782; Percent Effort: 5%; Total Award Period Covered: 1/2009–1/2011; Support: completed.
- 40) **2010 ACS SEED Program at CWRU**; PI: Crespo; Source of Support: ACS; Total Award Amount: \$13,200; Total Direct Costs: \$13,200; Percent Effort: 2%; Total Award Period Covered: 7/2010–6/2011; Support: **completed**.
- 41) Binding of DNA and Amino Acids Components to Nitrogen-Rich Compounds (DoD-W912HZ-09-P-0096); PI: Crespo; Source of Support: DoD/USACE-Army Corps of Engineers; Total Amount: \$40,000; Total Direct Costs: \$25,478; Percent Effort: 5%; Total Award Period Covered: 1/2009–12/2009; Support: completed.
- 42) Photochemical Fate of Organic Pollutants in the Aquatic Environments; PI: Crespo; Source of Support: ACES Opportunity Grant; Total Amount: \$20,000; Total Direct Costs: \$20,000; Percent Effort: 2%; Total Award Period Covered: 1/2008-8/2008; Support: completed.
- 43) Ground and Excited State Calculations of Organic Molecules; PI: Crespo; Source of Support: Mississippi Center for Supercomputer Research; Total Award Amount: 300,000 RUs; Total Direct Costs: 300,000 RUs; Percent Effort: 0%; Total Award Period Covered: 8/2007–7/2015; Support: completed.

**Collaborators and Co-editors** (during the past 5 years)

- Rafael Arce, Department of Chemistry, University of Puerto Rico, San Juan, Puerto Rico, USA
- Antonio Carlos Borin, Department of Fundamental Chemistry, Institute of Chemistry, University of São Paulo, São Paulo, Brazil
- Inés Corral, Department of Chemistry, Autonomous University of Madrid, Madrid, Spain
- Ganglong Cui, Department of Chemistry, Beijing Normal University, Beijing, China
- Leticia González, Institute for Theoretical Chemistry, University of Vienna, Vienna, Austria
- Jesús González-Vázquez, Department of Chemistry, Autonomous University of Madrid, Madrid, Spain
- Leonid Gorb, Department of Molecular Biophysics, Institute of Molecular Biology and Genetics, National Academy of Science of Ukraine, Kyiv, Ukraine
- Thomas Gustavsson, LIDYL, CEA, CNRS, Université Paris-Saclay, F-91191 Gif-sur-Yvette, France
- Eckhard Jankowsky, Department of Biochemistry, Case Western Reserve University School of Medicine, Cleveland, Ohio, USA
- Steffen Jockusch, Department of Chemistry, Columbia University, New York City, New York, USA
- Minh Lam, Department of Dermatology, Case Western Reserve University School of Medicine, Cleveland, Ohio, USA
- Maurizio Persico, Department of Chemistry and Industrial Chemistry, University of Pisa, Pisa, Italy
- Michael Pittelkow, Department of Chemistry, University of Copenhagen, Copenhagen, Denmark
- Geneviève Sauvé, Department of Chemistry, Case Western Reserve University, Cleveland, Ohio, USA
- Theis I. Sølling, Department of Chemistry, University of Copenhagen, Copenhagen, Denmark
- Blanton Tolbert, Department of Chemistry, Case Western Reserve University, Cleveland, Ohio, USA
- Yitzhak Tor, Department of Chemistry, University of California, San Diego, California, USA
- Susanne Ullrich, Department of Physics and Astronomy, University of Georgia, Athens, Georgia, USA
- Han Xiao, Department of Chemistry, Rice University, Houston, Texas, USA
- Jianzhang Zhao, School of Chemical Engineering, Dalian University of Technology, Dalian, China

### Publications (\* = corresponding author)

**Note on Discipline's Convention for Order of Authorship:** Authors appear in decreasing order of intellectual contribution, except for the corresponding author, who usually is assigned the last position.

### Peer-Reviewed Publications done at CWRU (Google Scholar: +9,253 citations; h-index 43, i10-index 84) <sup>†</sup> Participated as undergraduate student; <sup>‡</sup> Participated as high school student.

- Khan, R. R.; Seth, S. K.; Mathew, R.; Falcón-Cruz, N. V.; Acquah, C.; Jockusch, S.; Levi, L.; Crespo-Hernández, C. E. "Alloxazine derivatives as multifunctional agents for photodynamic therapy, cancer cell imaging, and cell proliferation inhibition", **2025**, *submitted*.
- 2) Feierabend, K.; Allison, J. M.; Olson, K. S.; Bowers, B. B.; Hoehn, S. J.; Krul, S. E.; Crespo-Hernández, C. E. "Photochemistry of Aqueous Warfarin and 4-Hydroxycoumarin", **2025**, *submitted*.
- Seth, S. K.; Acquah, C.; Levi, L.; Jockusch, S.; Crespo-Hernández, C. E. "Harnessing the Excited States of 5-(5-Phenylthiophen-2-yl)-6-Azauridine as a Three-Pronged Agent for Skin Cancer Therapy: Photodynamic Action, Cell Imaging, and Cancer Cell Inhibition", ACS Applied Bio Materials 2025, DOI: 10.1021/acsabm.5c01035.
- Hoehn, S. J.; Krul, S. E.; Acquah, C.; Crespo-Hernández, C. E. "Impact of Diamino and Imidazole Functionalization on the Photophysical Properties and Electronic and Structural Dynamics of the Pyrimidine Nucleobase" (Invited Manuscript), *J. Chem. Phys.* 2025, in press.
- 5) Acquah, C.; Seth, S. K.; Feng, C.; Jockusch, S.; Levi, L.; Falcón-Cruz, N. V.; Li, L.; Crespo-Hernández, C. E. "dTAT1: An Unnatural Nucleoside Exhibiting Low Photocytotoxicity for Genetic Code Expansion", *J. Phys. Chem. Lett.* **2025**, 16, 5390-5397.

### Highlighted with the journal's Front Cover.

- 6) Hoehn, S. J.; Krul, S. E.; Seth, S. K.; Crespo-Hernández, C. E. "Structure-Photophysical Property Relationships in Non-Canonical and Synthetic Nucleobases" (Invited Review), *Annu. Rev. Phys. Chem.* **2025**, vol. 76, 539-564.
- 7) Mai, S.; Ashwood, B.; Marquetand, P; Crespo-Hernández, C. E.; González, L., "Correction to <u>"Solvatochromic Effects on the Absorption Spectrum of 2-Thiocytosine"</u>, *J.Phys. Chem. B* **2024**, 128, 12668.
- Griffith, C.; Krul, S. E.; Hoehn, S. J.; Phan, T.; Crespo-Hernández, C. E. "Structural and Electronic Factors Controlling the Efficiency and Rate of Intersystem Crossing to the Triplet State in Thiophene Polycyclic Derivatives", *Chem. Eur. J.* 2024, e202402721 (1 of 10).

# Selected as a "Hot Paper". Hot Papers are chosen by the Editors for their importance in a rapidly evolving field of high current interest.

- Griffith, C.; Mao, E.; Hoehn, S. J.; Krul, S. E.; Crespo-Hernández, C. E. "Carbon-Sulfur Bond Elongation as the Promoting Reaction Coordinate in the Efficient Sub-Nanosecond Intersystem Crossing in Thianaphthene Derivatives", *Phys. Chem. Chem. Phys.* 2024, 26, 23457-23467.
- Acquah, C.; Hoehn, S. J.; Krul, S. E.; Jockusch, S.; Yang, S.; Seth, S. K.; Lee, E.; Xiao, H.; Crespo-Hernández, C. E.,\* "Electronic Relaxation Pathways in Thio-Acridone and Thio-Coumarin: Two Heavy-Atom-Free Photosensitizers Absorbing Visible Light", *Phys. Chem. Chem. Phys.* 2024, 26, 28980-28991.
- 11) Valverde, D.; Hoehn, S. J.; Koyanagui, E. D.; Krul, S. E.; Crespo-Hernández,\* C. E.; Borin, A. C.,\* "Theoretical and experimental evaluation of the electronic relaxation mechanisms of 2-pyrimidinone: the primary UVA absorbing moiety in DNA and RNA (6-4) photolesion", *ChemPhotoChem* **2024**, 8(12), e202400070 (1 of 13).
- 12) Acquah, C.; Pabis, Z.;<sup>†</sup> Seth, S. K.; Levi, L.; Crespo-Hernández, C. E.,<sup>\*</sup> "Low Cost, 3D Printed Irradiation System for In Vitro Photodynamic Therapy Experiments", *Photochem. Photobiol.* **2024**, 100, 530-540.

Selected by the American Photobiology Society as "Jornal Article of the Month" and featured on their LinkedIn site as <u>"A fascinating new journal study"</u>.

# Among the Mos-Read Papers in Photochemistry and Photobiology between January 2023 to December 2023.

13) Crespo-Hernández, C. E. "Editorial: Special issue on nucleic acid photophysics", *Photochem. Photobiol.* **2024**, 100, 257-261.

### Highlighted in the journal's Front Cover.

- 14) S. Beiharz;<sup>†</sup> M. Vermut-Young;<sup>†</sup> K. Anderson;<sup>‡</sup> D. Vinella; A. Pahuja; Y. Yuan; K. Raheja; C. E. Crespo-Hernández; M. Karayilan,<sup>\*</sup> "Summer Research Plan in Polymer Chemistry Laboratory for ACS Project SEED Program", *J. Chem. Ed.* **2024**, 101, 1120-1129.
- 15) E. Finol;\* S. E. Krul; S. J. Hoehn; C. E. Crespo-Hernández,\* "The mRNACalc web server accounts for the hypochromicity of modified nucleosides and enables the accurate quantification of nucleoside-modified mRNA", *Mol. Ther. Nucleic Acids* **2024**, 35, 1-7.
- 16) L. A. Ortiz-Rodríguez; N. E. Caldero-Rodríguez; S. K. Seth; K. Díaz-González; C. E. Crespo-Hernández, "Electronic Relaxation Mechanism of 9-Methyl-2,6-Diaminopurine and 2,6-Diaminopurine-2'-Deoxyribose in

Solution", Photochem. Photobiol. 2024, 100, 393-403.

Invited Manuscript; submitted as part of the Special Issue on Nucleic Acid Photophysics.

 S. J. Hoehn; S. E. Krul; M. M. Pogharian;<sup>†</sup> E. Mao; C. E. Crespo-Hernández,<sup>\*</sup> "Photochemical Stability of 5-Methylcytidine Relative to Cytidine: Photophysical Insight for mRNA Therapeutic Applications", *J. Phys. Chem. Lett.* 2023, 14, 10856-10862.

Highlighted in the journal's Front Cover.

- 18) L. A. Ortiz-Rodríguez; Y.-G. Fang; G. Niogret; K. Hadidi; S. J. Hoehn; H. J. Folkwein; S. Jockusch; Y. Tor;\* G. Cui;\* L. Levi;\* C. E. Crespo-Hernández,\* "Thieno[3,4-d]pyrimidin-4(1H)-thione: An Effective, Oxygenation Independent, Heavy-Atom-Free Photosensitizer for Cancer Cells", *Chem. Sci.* 2023, 14, 8831-8841.
- C. Griffith; S. E. Krul; S. J. Hoehn; E. Mao; G. Sleyko;<sup>†</sup> C. E. Crespo-Hernández,<sup>\*</sup> "Excited State Dynamics of Dibenzothiophene Derivatives", *J. Phys. Chem. B* 2023, 127, 5924–5932.
- 20) S. E. Krul; G. J. Costa; S. J. Hoehn; D. Valverde; L. M. F. Olivera; A. C. Borin;\* C. E. Crespo-Hernández,\* "Resolving Ultrafast Photoinitiated Dynamics of the Hachimoji 5-Aza-7-Deazaguanine Nucleobase: Impact of Synthetically Expanding the Genetic Alphabet", *Photochem. Photobiol.* **2023**, 99, 693-705.

Invited Manuscript; submitted as part of the Special Issue celebrating the 50<sup>th</sup> Anniversary of the American Society for Photobiology.

Highlighted by: M. S. de Vries, "Understanding How a New Hachimoji Nucleobase Alters Photodynamics of Genetic Building Blocks", *Photochem. Photobiol.* **2023**, 99, 857-859.

- J. Ortín-Fernández; N. E. Caldero-Rodríguez; E. M. Arpa; C. E. Crespo-Hernández; L. Martínez-Fernández; I. Corral, "Photophysical Characterization of Isoguanine in a Prebiotic-Like Environment", *Chem. Eur. J.* 2023, 29, e202203580.
- N. E. Caldero-Rodríguez; E. M. Arpa; D. Cárdenas; L. Martínez-Fernández; I. Corral; C. E. Crespo-Hernández,\* "2-Oxopurine Riboside: A Dual Fluorescent Analog and Photosensitizer for RNA/DNA Research", *J. Phys. Chem. B* 2022, 126, 4483-4490.
- 23) E. Vos; S. J. Hoehn; S. Krul; C. E. Crespo-Hernández,\* J. González-Vázquez;\* I. Corral,\* "Disclosing the role of C4-oxo substitution in the photochemistry of DNA and RNA pyrimidine monomers: Formation of photoproducts from the vibrationally-excited ground state", *J. Phys. Chem. Lett.* **2022**, 13, 2000-2006.
- 24) N. E. Caldero-Rodríguez; C. E. Crespo-Hernández,\* "Excited State Dynamics of 2'-Deoxyisoguanosine and Isoguanosine in Aqueous Solutions", *Phys. Chem. Chem. Phys.* **2022**, 24, 6769-6781.
- 25) L. A. Ortiz-Rodríguez; Hoehn, S. J.; C. E. Crespo-Hernández,\* "On the Photostability of Cyanuric Acid and its Candidature as a Prebiotic Nucleobase", *Molecules* 2022, 27(4), 1184.

Invited Manuscript; submitted as part of the Special Issue "Ultrafast Dynamics in Chemical Processes".

26) N. E. Caldero- Rodríguez; Ortiz- Rodríguez; L. A.; Gonzalez, A. A.;<sup>†</sup> C. E. Crespo-Hernández,<sup>\*</sup> "Photostability of 2,6-Diaminopurine and its 2'-Deoxyriboside Investigated by Femtosecond Transient Absorption Spectroscopy", *Phys. Chem. Chem. Phys.* 2022, 24, 4204-4211.

### Highlighted by the editors of PCCP as one of the hottest papers published in 2022.

- 27) S. J. Hoehn; S. E. Krul; B. J. Skory;<sup>†</sup> C. E. Crespo-Hernández,<sup>\*</sup> "Increased Photostability of the Integral mRNA Vaccine Component N1-Methylpseudouridine Compared to Uridine", *Chem. Eur. J.* **2022**, 28, e202103667.
- 28) L. A. Ortiz-Rodríguez; G. Ortiz-Zayas; M. Pollum; S. Jockusch; C. E. Crespo-Hernández,\* "Photochemistry of the Thiopurine Prodrugs: Intramolecular Charge Recombination in Azathioprine Quenches the Population of the Reactive Triplet State in 6-Mercaptopurine", *Photochem. Photobiol.* **2022**, 98, 617-632.

This paper is part of the P&P Special Issue Honoring Prof. Jean Cadet's research contributions.

29) L. A. Ortiz-Rodríguez; S. J. Hoehn; C. Acquah; N. Abbass;<sup>†</sup> L. Waidmann;<sup>†</sup> C. E. Crespo-Hernández,<sup>\*</sup> "Femtosecond Intersystem Crossing to the Reactive Triplet State of the 2,6-Dithiopurine Skin Cancer Photosensitizer", *Phys. Chem. Chem. Phys.* **2021**, 23, 25048-25055.

### Highlighted by the editors of PCCP as one of the hottest papers published in 2021.

 D. Sharma; L. L. Zagore; M. M. Brister; X. Ye; C. E. Crespo-Hernández; D. D. Licatalosi,\* E. Jankowsky,\* "The Kinetic Landscape of an RNA Binding Protein in Cells", *Nature* 2021, 591, 152–156.

Highlighted in Nature magazine News and Views.

### Highlighted among other news media by:

(1) <u>EurekAlert!</u>; (2) <u>Newswise</u>; (3) <u>Mirage News</u>; (4) <u>Sciencenewsnet</u>; (5) <u>Science Magazine</u>; (6) <u>Medical</u> <u>News</u>; (7) <u>Phys.org</u>; (8) <u>AZO Life Sciences</u>.

- L. A. Ortiz-Rodríguez; S. J. Hoehn; A. Loredo; L. Wang; H. Xiao; C. E. Crespo-Hernández,\* "Thionated Organic Compounds as Emerging Heavy-Atom-Free Photodynamic Therapy Agents", *J. Am. Chem. Soc.* 2021, 143, 7, 2676–2681.
- 32) S. E. Krul; S. J. Hoehn; K. Feierabend; C. E. Crespo-Hernández,\* "Excited State Dynamics of 7-Deazaguanosine and Guanosine 5' Monophosphate", *J. Chem. Phys.* **2021**, 154, 075103.
- 33) L. A. Ortiz-Rodríguez; C. Reichardt; S. J. Hoehn; S. Jockusch; C. E. Crespo-Hernández,\* "Detection of the Thietane Intermediate in the UVA-Induced Formation of the (6-4) Photoadduct in DNA", *Nature Communications*, 2020, 11, 3599.

### Featured by the editors of Nature Communications in a dedicated Editors' Highlights webpage.

### Highlighted among other news media by:

(1) *EurekAlert!*; (2) *The Daily*; (3) *Medical Xpress*; (4) *ecancer*; (5) *Science Magazine*; (6) *Medical News*.

- 34) L. A. Ortiz-Rodríguez; C. E. Crespo-Hernández,\* "Thionated Organic Compounds as Emerging Heavy-Atom-Free Photodynamic Therapy Agents", *Chem. Sci.* 2020, 11, 11113-11123. (Invited Minireview, highlighted in the journal's inside <u>Back Cover</u>)
- 35) E. M. Arpa; M. M. Brister; S. J. Hoehn; C. E. Crespo-Hernández;\* I. Corral,\* "On the Origin of the Photostability of DNA and RNA Monomers: Excited State Relaxation Mechanism of the Pyrimidine Chromophore", *J. Phys. Chem. Lett.* **2020**, 11, 5156-5161.
- 36) M. M. Brister; T. Gustavsson;\* C. E. Crespo-Hernández,\* "Radiative Decay Lifetimes of Sulfur-Substituted DNA

and RNA Monomers Measured Using the Femtosecond Fluorescence Up-Conversion Technique", *Molecules*, **2020**, 25, 584 (16 pages).

Invited Manuscript; submitted as part of the themed issue on the "Fluorescence Spectroscopy of Biomolecules".

 L. Martínez-Fernández; S. Arslancan; D. Ivashchenko; C. E. Crespo-Hernández; I. Corral,\* "Tracking the Origin of Photostability in Purine Nucleobases: the Photophysics of 2-Oxopurine", *Phys. Chem. Chem. Phys.* 2019, 21, 13467-13473.

*Highlighted by the editors of PCCP* as one of the hottest papers published in the journal in 2019. Access full the collection <u>here</u>.

- 38) M. M. Brister; C. E. Crespo-Hernández,\* "Excited-State Dynamics in the RNA Nucleotide Uridine 5'-Monophosphate Investigated using Femtosecond Broadband Transient Absorption Spectroscopy", J. Phys. Chem. Lett. 2019, 10, 2156-2161.
- 39) M. Ashfold; S. Bai; S. Bradforth; P. Chabera; J. Cina; C. E. Crespo-Hernández; et al., "Photo-Protection/Phot-Damage in Natural Systems: General Discussion", *Faraday Discuss.* **2019**, 216, 538-563.
- 40) M. Ashfold; J. Bender; E. Bittner; J. Cina; C. E. Crespo-Hernández; et al., "Photovoltaics and Bio-Inspired Light Harvesting: General Discussion", *Faraday Discuss.* **2019**, 216, 269-300.
- 41) Ashwood, B.;<sup>†</sup> Pollum, M.; Crespo-Hernández, C. E.,\* "Photochemical and Photodynamical Properties of Sulfur-Substituted Nucleic Acid Bases", *Photochem. Photobiol.* **2019**, 95, 33-58. Invited Review; submitted as part of the Special Issue honoring the 55th Anniversary of Photochemistry and Photobiology.

Highlighted by Wiley among the top 20 downloaded papers in P&P during January 2017 to December 2018.

Highlighted by Wiley among the top cited papers in P&P during January 2018 to December 2019.

- 42) K. Farrell;<sup>†</sup> M. Pillelkow; T. I. Sølling; C. E. Crespo-Hernández,<sup>\*</sup> "Enhanced Ultrafast Intersystem Crossing Dynamics in 6-Selenoguanine Compared to 6-Thioguanine ", *J. Am. Chem. Soc.* **2018**, *140*, 11214-11218.
- 43) M. Pollum; L. Minh; S. Jockusch; C. E. Crespo-Hernández,\* "Dithionated Nucleobases as Effective Photodynamic Agent Against Human Epidermoid Carcinoma Cells", *ChemMedChem* **2018**, 13, 1044-1050.

Selected by the editors of Wiley as part of a Virtual Issue titled "*MedChem in the USA*". Access the collection <u>here.</u>

44) R. DiScipio; G. Sauvé;\* C. E. Crespo-Hernández,\* "Photodynamics in Metal Chelating Tetraphenylazadipyrromethene Complexes: Implications for Their Potential Use as Photovoltaic Materials", J. Phys. Chem. C 2018, 122, 13579-13589.

Invited Manuscript; submitted as part of the themed collection honoring Prof. Prashant V. Kamat Festschrift.

45) B. Ashwood;<sup>†</sup> L. A. Ortiz-Rodríguez; C. E. Crespo-Hernández,<sup>\*</sup> "Photochemical Relaxation Pathways of S<sup>6</sup>-Methylthioinosine and O<sup>6</sup>-Methylguanosine in Solution", *Faraday Discuss.* **2018**, 207, 351-374.

Invited Manuscript; submitted as part of the "Photoinduced Processes in Nucleic Acids and Proteins:

### Faraday Discussion".

- 46) A. Chandra; R. Cogdell; C. E. Crespo-Hernández, et al., "Light Induced Damage and Repair in Nucleic Acids and Proteins: General Discussion", *Faraday Discuss.* **2018**, 207, 389-408.
- 47) V. Bhat; R. Cogdell; C. E. Crespo-Hernández, et al., "Photocrosslinking between Nucleic Acids and Proteins: General Discussion", *Faraday Discuss.* **2018**, 207, 283-306.
- 48) A. Chattopadhyay; R. Cogdell; C. E. Crespo-Hernández, et al., "Light Induced Charge and Energy Transport in Nucleic Acids and Proteins: General Discussion", *Faraday Discuss.* **2018**, 207, 153-180.
- B. Ashwood;<sup>†</sup> L. A. Ortiz-Rodríguez; C. E. Crespo-Hernández,<sup>\*</sup> "Excited-State Dynamics of O6-Methylguanosine: Impact of O6-Methylation on the Photophysics of Guanine Monomers", *J. Phys. Chem. Lett.* 2017, 8, 4380-4385.
- 50) W. Yang; B. Ashwood;<sup>†</sup> J. Zhao;<sup>\*</sup> W. Ji; D. Escudero; D. Jacquemin;<sup>\*</sup> C. E. Crespo-Hernández,<sup>\*</sup> "Ultrafast Excited-State Dynamics in Cyclometalated Ir(III) Complexes Coordinated with Perylenebisimide and Its π-Radical Anion Ligands", *J. Phys. Chem. C* **2017**, 121, 21184-21198.
- 51) M. M. Brister; L. E. Piñero-Santiago; M. Morel; R. Arce;\* C. E. Crespo-Hernández,\* "Photochemical Relaxation Pathways in Dinitropyrene Isomer Pollutants", *J. Phys. Chem. A* **2017**, 121, 8197-8206.
- 52) M. Tolbert; C. E. Morgan; M. Pollum; C. E. Crespo-Hernández; Mei-Ling Li;\* G. Brewer;\* B. S. Tolbert,\* "HnRNP A1 Alters the Structure of a Conserved Enterovirus IRES Domain to Stimulate Viral Translation", *J. Mol. Biol.* 2017, 429, 2841-2858. (Featured Article)

### Highlighted by:

Schroeder, S. J., "Stack Locally and Act Globally: A Few Nucleotides Make All the Difference in Enterovirus 71 IRES Binding hnRNAP A1 and Infectious Phenotypes: Commentary on "HnRNP A1 Alters the Structure of a Conserved Enterovirus IRES Domain to Stimulate Viral Translation", J. Mol. Biol. **2017**, 429, 2859-2862.

53) J. A. Sánchez-Rodríguez; A. Mohamadzade; S. Mai; B. Ashwood;<sup>↑</sup> M. Pollum; P. Marquetand; L. González;<sup>\*</sup> C. E. Crespo-Hernández;<sup>\*</sup> S. Ullrich,<sup>\*</sup> "2-Thiouracil Intersystem Crossing Photodynamics Studied by Wavelength-Dependent Photoelectron and Transient Absorption Spectroscopies", *Phys. Chem. Chem. Phys.* 2017, 19, 19756-19766.

Invited Manuscript; submitted as part of the themed issue on the "XUV/X-Ray Light and Fast lons for Ultrafast Chemistry".

54) R. DiScipio; R. Y. Santiago;<sup>†</sup> D. Taylor;<sup>‡</sup> C. E. Crespo-Hernández,<sup>\*</sup> "Electronic Relaxation Pathways of the Biologically Relevant Pterin Chromophore", *Phys. Chem. Chem. Phys.* **2017**, 19, 12720-12729.

Highlighted by the editors of PCCP as one of the hottest papers published in 2017. Access the collection here.

- 55) S. Mai; B. Ashwood;<sup>†</sup> P. Marquetand; C. E. Crespo-Hernández;<sup>\*</sup> L. González,<sup>\*</sup> "Solvatochromic Effects on the Absorption Spectrum of 2-Thiocytosine", *J. Phys. Chem. B* **2017**, 121, 5187-5196.
- 56) B. Ashwood;<sup>†</sup> S. Jockusch; C. E. Crespo-Hernández,<sup>\*</sup> "Photochemical Reactivity of dTPT3: A Crucial Nucleobase Derivative in the Development of Semi-Synthetic Organisms", *J. Phys. Chem. Lett.* **2017**, 8,

2387-2392.

57) C. E. Crespo-Hernández,\* "Photorelaxation and Photorepair Processes in Nucleic and Amino Acid Derivatives", *Molecules* **2017**, 22, 2203.

Editorial submitted as part of the themed issue on the "Experimental and Computational Photochemistry of Bioorganic Molecules".

58) B. Ashwood;<sup>†</sup> S. Jockusch; C. E. Crespo-Hernández,<sup>\*</sup> "Excited-State Dynamics of the Thiopurine Prodrug 6-Thioguanine: Can N9-Glycosylation Affects Its Phototoxic Activity?", *Molecules* **2017**, 22, 379 (15 pages).

Invited Manuscript; submitted as part of the themed issue on the "Experimental and Computational Photochemistry of Bioorganic Molecules".

59) L. Martínez-Fernández; G. Granucci; M. Pollum; C. E. Crespo-Hernández;\* M. Persico;\* I. Corral,\* "Decoding the Molecular Basis for the Population Mechanism of the Triplet Phototoxic Precursors in UVA Light-Activated Pyrimidine Anticancer Drugs", *Chem. Eur. J.* 2017, 23, 2619-2627.

**Highlighted by:** *Clarivate Analytics* (previously, Thomson Reuters Web of Science) as a '*Highly Cited Paper*' in 2017.

- 60) M. M. Brister; L. E. Piñero-Santiago; M. Morel; R. Arce;\* C. E. Crespo-Hernández,\* "The Photochemical Branching Ratio in 1,6-Dinotropyrene Depends on Excitation Energy", *J. Phys. Chem. Lett.* **2016**, 7, 5086-5092.
- S. Mai; M. Pollum; L. Martínez-Fernández; N. Dunn; P. Marquetand; I. Corral;\* C. E. Crespo-Hernández;\* L. González,\* "The Origin of Efficient Triplet State Population in Sulfur-Substituted Nucleobases", *Nature Commun.* 2016, 7, 13077 (8 pages).
- 62) B. Ashwood;<sup>†</sup> M. Pollum; C. E. Crespo-Hernández,<sup>\*</sup> "Can a Six-Letter Alphabet Increase the Likelihood of Photochemical Assault to the Genetic Code?", *Chem. Eur. J.* **2016**, 22, 16648-16656.
- 63) M. Pollum; B. Ashwood;<sup>†</sup> S. Jockusch; M. Lam, C. E. Crespo-Hernández,<sup>\*</sup> "Unintended Consequences of Expanding the Genetic Alphabet", *J. Am. Chem. Soc.* **2016**, 138, 11457-11460.

# Highlighted by the American Chemical Society Office of Public Affairs' Weekly Press PACs; Nature's Research Highlights; Phys.org, among other news media:

American Chemical Society Office of Public Affairs' Weekly Press PACs.

Nature magazine in <u>Research Highlights</u>.

Newswise An Expanded genetic code is shown phototoxic to cells.

PHYS.ORG Unintended consequences of creating the world's first semisynthetic organism.

MedicalResearch.com Expanded Genetic DNA more Susceptible to Ultraviolet Light Damage.

- M. Pollum; L. Guan; S. Ahsanuddin; E. Baron; M. Lam; C. Crespo-Hernández,\* "Photoactivation of sulfurmodified DNA and RNA analogs induces cytotoxicity in epidermoid carcinoma cells", *J. Invest. Dermatol.* 2016, 136, S105.
- 65) H. Yu; J. A. Sanchez-Rodriguez; S. Ullrich;\* M. Pollum; C. E. Crespo-Hernández; S. Mai.; P. Marquetand; L.

González, "Internal Conversion and Intersystem Crossing Pathways in UV Excited, Isolated Uracils and Their Implications in Prebiotic Chemistry", *Phys. Chem. Chem. Phys.* **2016**, 18, 20168-20176.

Invited Manuscript; submitted as part of the themed issue on the "Prebiotic Chemistry and the Molecular Origins of Life".

 M. Brister; M. Pollum; C. E. Crespo-Hernández,\* "Photochemical Etiology of Promising Ancestors of the RNA Nucleobases", *Phys. Chem. Chem. Phys.* 2016, 18, 20097-20103.

Invited Manuscript; submitted as part of the themed issue on the "Prebiotic Chemistry and Molecular Origins of Life".

### Highlighted in the journal's **Back Cover**.

 M. Pollum; L. A. Ortiz-Rodríguez;<sup>†</sup> S. Jockusch; C. E. Crespo-Hernández,<sup>\*</sup> "The Triplet State of 6-Thio-2'deoxyguanosine: Intrinsic Properties and Reactivity toward Molecular Oxygen", *Photochem. Photobiol.* 2016, 92, 286-292.

Selected as one of the top papers published in the journal Photochemistry & Photobiology, as part a virtual issue celebrating its 55th anniversary.

- 68) M. Brister; C. E. Crespo-Hernández,\* "Direct Observation of Triplet-State Population Dynamics in the RNA Uracil Derivative 1-Cyclohexyluracil", *J. Phys. Chem. Lett.* **2015**, 6, 4404-4409.
- 69) M. Pollum; S. Jockusch; C. E. Crespo-Hernández,\* "Increase in the Photoreactivity of Uracil Derivatives by Doubling Thionation", *Phys. Chem. Chem. Phys.* **2015**, 17, 27851-27861.
- 70) C. E. Crespo-Hernández;\* L. Martínez-Fernández.; C. Rauer; C. Reichardt; S. Mai; M. Pollum; P. Marquetand; L. González;\* I. Corral,\* "Electronic and Structural Elements that Regulate the Excited-State Dynamics in Purine Nucleobase Derivatives", J. Am. Chem. Soc. 2015, 137, 4368-4381.
- 71) M. Pollum; S. Jockusch; C. E. Crespo-Hernández,\* "2,4-Dithiothymine as a Potent UVA Chemotherapeutic Agent", *J. Am. Chem. Soc.* 2014, 136, 17930-17933.
- 72) M. Pollum; C. E. Crespo-Hernández,\* "Communication: The Dark Singlet State as a Doorway State in the Ultrafast and Efficient Intersystem Crossing Dynamics in 2-Thiothymine and 2-Thiouracil", J. Chem. Phys. 2014, 140, 071101.
- 73) C. E. Crespo-Hernández,\* R. A. Vogt; Sealey, B.;<sup>‡</sup> "On the Primary Reaction Pathways in the Photochemistry of Nitro-Polycyclic Aromatic Hydrocarbons", *Mod. Chem. Appl.* **2013**, 1, 106.
- 74) R. A. Vogt; C. E. Crespo-Hernández,\* "Conformational Control in the Population of the Triplet State and Photoreactivity of Nitronaphthalene Derivatives ", J. *Phys. Chem. A* **2013**, 117, 14100-14108.
- 75) T. Fujiwara;\* C. Reichardt; R. A. Vogt; C. E. Crespo-Hernández; M. Z. Zgierski; E. C. Lim, "Electronic Spectra and Excited-State Dynamics of 4-Fluoro-*N*,*N*-dimethylaniline", *Chem. Phys. Lett.* **2013**, 586, 70-75.
- 76) R. A. Vogt; C. Reichardt; C. E. Crespo-Hernández,\* "Excited-State Dynamics in Nitro-Naphthalene Derivatives: Intersystem Crossing to the Triplet Manifold in Hundreds of Femtoseconds", J. Phys. Chem. A 2013, 117, 6580-6588.

77) C. Reichardt; C. Wen; R. A. Vogt; C. E. Crespo-Hernández,\* "Role of Intersystem Crossing in the Fluorescence Quenching of 2-Aminopurine 2'-deoxyriboside in Solution", *Photochem. Photobiol. Sci.* **2013**, 12, 1341-1350.

Invited Manuscript; submitted as part of the themed issue on the "Interaction of UV Radiation with DNA".

- 78) R. A. Vogt; T. G. Gray;\* C. E. Crespo-Hernández,\* "Subpicosecond Intersystem Crossing in Mono- and Di-(Organophosphine)gold(I) Naphthalene Derivatives in Solution", *J. Am. Chem. Soc.* **2012**, 134, 14808–14817.
- 79) O. Isayev;\* C. E. Crespo-Hernández; L. Gorb; F. C. Hil; J. Leszczynski; "In Silico Structure-Function Analysis of E. cloacae Nitroreductase", *Proteins* **2012**, 80, 2728-2741.
- 80) C. Reichardt; C. Guo; C. E. Crespo-Hernández,\* "Excited-State Dynamics in 6-Thioguanosine from the Femtosecond to Microsecond Time Scale", *J. Phys. Chem. B* **2011**, 115, 3263-3270.
- L. G. Dodosn;<sup>†</sup> R. A. Vogt; J. Marks;<sup>†</sup> C. Reichardt; C. E. Crespo-Hernández,<sup>\*</sup> "Photophysical and Photochemical Properties of the Pharmaceutical Compound Salbutamol in Aqueous Solutions", *Chemosphere* 2011, 83, 1513-1523.
- 82) J. Santos-Pérez;\* C. E. Crespo-Hernández;\* C. Reichardt; C. R. Cabrera; I. Feliciano-Ramos; L. Arroyo-Ramírez; M. A. Meador,\* "Synthesis, Optical Characterization, and Electrochemical Properties of Isomeric Tetraphenylbenzodifurans Containing Electron Acceptor Groups", *J. Phys. Chem. A* 2011, 115, 4157-4168.
- 83) Y. Díaz-Espinosa; C. E. Crespo-Hernández; A. E. Alegría;\* C. García; R. Arce,\* "Quenching Enhancement of the Singlet Excited State of Pheophorbide-a by DNA in the Presence of the Quinone Carboquone", *Photochem. Photobiol.* 2011, 87, 275-283.
- 84) C. Reichardt; C. E. Crespo-Hernández,\* "Room-Temperature Phosphorescence of the DNA Monomer Analogue 4-Thiothymidine after UVA Excitation", *J. Phys. Chem. Lett.* **2010**, 1, 2239-2243.
- 85) C. Reichardt; C. E. Crespo-Hernández,\* "Ultrafast Spin Crossover in 4-Thiothymidine in an Ionic Liquid", *Chem. Commun.* **2010**, 46, 5963-5965.
- 86) R. A. Vogt; M. A. Peay; T. G. Gray;\* C. E. Crespo-Hernández,\* "Excited-State Dynamics of (Organophosphine)Gold(I) Pyrenyl Isomers", J. Phys. Chem. Lett. 2010, 1, 1205-1211.
- 87) C. Reichardt; R. A. Vogt; C. E. Crespo-Hernández,\* "On the Origin of Ultrafast Nonradiative Transitions in Nitro-PAHs: Excited-State Dynamics in 1-Nitronaphthalene", *J. Chem. Phys.* **2009**, 131, 224518 (*15 pages*).
- D. M. Close; C. E. Crespo-Hernández;\* L. Gorb; J. Leszczynski," Ionization Energy Thresholds of Microhydrated Adenine and Its Tautomers", J. Phys. Chem. A 2008, 112, 12702-12706.
- 89) C. E. Crespo-Hernández;\* Burdzinski, G.; R. Arce, "Environmental Photochemistry of Nitro-PAHs: Direct Observation of Ultrafast Intersystem Crossing in 1-Nitropyrene", *J. Phys. Chem. A* **2008**, 112, 6313-6319.
- 90) D. M. Close,\* C. E. Crespo-Hernández;\* L. Gorb; J. Leszczynski, "Theoretical Elucidation of Conflicting Experimental Data on Vertical Ionization Potentials of Microhydrated Thymine", *J. Phys. Chem. A* 2008, 112, 4405-4409.

### Before joining CWRU

91) K. de La Harpe; C. E. Crespo-Hernández; B. Kohler,\* "Deuterium Isotope Effect on Excited-State Dynamics in

an Alternating GC Oligonucleotide", J. Am. Chem. Soc. 2009, 131, 17557-17559.

- 92) C. T. Middleton; K. de La Harpe; C. Su; Y. K. Law; C. E. Crespo-Hernández; B. Kohler,\* "DNA Excited-State Dynamics: From Single Bases to the Double Helix", *Annu. Rev. Phys. Chem.* **2009**, 60, 217-239. (**Review**)
- 93) K. de La Harpe; C. E. Crespo-Hernández; B. Kohler,\* "Excited-State Lifetimes in a G·C DNA Duplex are Nearly Independent of Helix Conformation and Base Pairing Motif", *ChemPhysChem* **2009**, 60, 1421-1425.

Invited Manuscript; submitted as part of the themed issue on the "Special Issue in Biophysics ".

- 94) C. E. Crespo-Hernández; K. de La Harpe; B. Kohler,\* "Ground-State Recovery Following UV Excitation is Much Slower in G-C-DNA Duplexes and Hairpins Than in Mononucleotides", J. Am. Chem. Soc. 2008, 130, 10844-10845.
- 95) Y. K. Law; J. Azadi;<sup>†</sup> C. E. Crespo-Hernández; E. Olmon;<sup>†</sup> B. Kohler; "Prediction of Thymine Dimerization Yields from Molecular Dynamics Simulations", *Biophysical J.* 2008, 94, 3590-3600.
- 96) T. Takaya; C. Su; K. de La Harpe; C. E. Crespo-Hernández; B. Kohler,\* "UV Excitation of DNA and RNA Strands Produces High yields of exciplex states between two stacked bases", *Proc. Natl. Acad. Sci. USA* 2008, 105, 10285-10290.
- 97) W. J. Schreier; T. E. Schrader; F. O. Koller; P. Gilch; C. E. Crespo-Hernández; V. N. Swaminathan; T. Carell; W. Zinth;\* B. Kohler,\* "Thymine Dimerization in DNA is an Ultrafast Photoreaction", *Science* **2007**, 315, 625-629.
- 98) P. M. Hare; C. E. Crespo-Hernández; B. Kohler,\* "Internal Conversion to the Electronic Ground State Occurs via Two Distinct Pathways for Pyrimidine Bases in Aqueous Solution", *Proc. Natl. Acad. Sci. USA* 2007, 104, 435-440.
- 99) C. E. Crespo-Hernández,\* D. M. Close; L. Gorb; J. Leszczynski, "Determination of Redox Potentials for the Watson-Crick Base Pairs, DNA Nucleosides, and Relevant Nucleosides Analogs", *J. Phys. Chem. B* 2007, 111, 5386-5395.
- C. E. Crespo-Hernández; B. Cohen; B. Kohler,\* "Molecular spectroscopy: Complexity of Excited-State Dynamics in DNA (Replay)", *Nature* 2006, 441, E7-E8.
- 101) D. M. Close;\* C. E. Crespo-Hernández;\* L. Gorb; J. Leszczynski, "The Influence of Microhydration on the Ionization Energy Thresholds of Thymine: Comparisons of Theoretical Calculations with Experimental Values", J. Phys. Chem. A 2006, 110, 7485-7490.
- 102) D. M. Close;\* C. E. Crespo-Hernández;\* L. Gorb; J. Leszczynski, "The Influence of Microhydration on the Ionization Energy Thresholds of Uracil and Thymine", *J. Phys. Chem. A* **2005**, 109, 9279-9283.
- 103) C. E. Crespo-Hernández; B. Cohen; B. Kohler,\* "Base Stacking Controls Excited-State Dynamics in A·Tcontaining DNA", *Nature* **2005**, 436, 1141-1144.
- 104) C. E. Crespo-Hernández; B. Cohen; P. M. Hare; B. Kohler,\* "Ultrafast Excited-State Dynamics in Nucleic Acids", *Chem. Rev.* 2004, 104, 1977-2019. (Review)
- 105) B. Cohen; C. E. Crespo-Hernández; B. Kohler,\* "Strickler-Berg Analysis of Excited Singlet State Dynamics in DNA and RNA Nucleosides", *J. Chem. Soc., Faraday Discuss.* **2004**, 127, 137-147.

- 106) C. E. Crespo-Hernández; B. Kohler,\* "Influence of Secondary Structure on Electronic Energy Relaxation in Adenine Homopolymers", *J. Phys. Chem. B* **2004**, 108, 11182-11188.
- 107) C. E. Crespo-Hernández,\* R. Arce;\* Y. Ishikawa; L. Gorb; J. Leszczynski; D. M. Close, "Ab Initio Ionization Energy Thresholds of DNA and RNA Bases in Gas Phase and in Aqueous Solution", J. Phys. Chem. A 2004, 108, 6373-6377.
- 108) C. E. Crespo-Hernández; R. Arce,\* "Formation of Formamidopyrimidine Nucleobase and Nucleoside as Major Products in the 254 nm Low-Intensity and 266 nm High-Intensity Irradiation of the Guanine Derivatives in Unbuffered Aqueous Solution", J. Photochem. Photobiol. B: Biol. 2004, 73, 167-175.
- 109) C. Crespo-Hernández; R. Arce; E. Quiñones,\* "Magnetic Field Enhancement of the 6-Methylpurine Photoionization Yield", *Chem. Phys. Lett.* **2003**, 382, 661-664.
- 110) C. E. Crespo-Hernández; R. Arce,\* "Near Threshold Photo-Oxidation of Dinucleotides Containing Purines upon 266 nm Nanosecond Laser Excitation. The Role of Bases Stacking, Conformation, and Sequence", J. Phys. Chem. B 2003, 107, 1062-1070.
- 111) C. E. Crespo-Hernández; R. Arce,\* "Photoionization of DNA and RNA Bases, Nucleosides and Nucleotides through a Combination of One- and Two-photon Pathways upon 266 nm Nanosecond Laser Excitation", *Photochem. Photobiol.* **2002**, 76, 259-267.
- 112) C. E. Crespo-Hernández; L. Martínez; A. E. González-Sierra; A. Díaz-Vázquez; R. Arce,\* "The 254 nm Low Intensity and 266 nm Laser Photochemistry of Adenosine. Effect of pH and Concentration on the Reactive Precursors of the Principal Products, Adenine and FAPyAde", *J. Photochem. Photobiol. A: Chem.* 2002, 152, 123-133.
- 113) E. E. Méndez; C. Crespo-Hernández; R. Figueroa; R. Arce; E. Quiñones,\* "Water Photoreduction Through the Direct Photoexcitation of Methylviologen", *J. Photochem. Photobiol. A: Chem.* **2001**, 142, 19-24.
- 114) C. E. Crespo-Hernández; R. Arce, "Part II. Mechanisms of Formation of Guanine as One of the Major Products in the 254 nm Photolysis of Guanine Derivatives: The Concentration and pH Effect", *Photochem. Photobiol.* **2000**, 71, 544-550.
- 115) C. E. Crespo-Hernández; S. Flores; C. Torres; I. Negrón-Encarnación; R. Arce,\* "Part I. Photochemical and Photophysical Studies of Guanine Derivatives: Intermediates Contributing to its Photodestruction Mechanism in Aqueous Solution and the Participation of the Electron Adduct", *Photochem. Photobiol.* 2000, 71, 534-543.
- 116) C. A. Reyes; M. Medina; C. E. Crespo-Hernández; M. Z. Cedeño; R. Arce,\* O. Rosario; M. E. Sigman;\* R. Dabestani, "The Photochemistry of Pyrene in Nonactivated Silica Gel Surfaces as a Model of Atmospheric Particulate", *Environ. Sci. Technol.* 2000, 34, 415-421.

### Book Chapters and Conference Proceedings Book Chapters

- 117) S. J. Hoehn, N. E. Caldero-Rodríguez.; C. E. Crespo-Hernández,\* "Photochemistry of RNA, RNA Monomers and their Plausible Prebiotic Precursors" (*Invited Review Chapter*), In *DNA Photodamage: From Light Absorption* to Cellular Responses and Skin Cancer; Douki, T.; Improta, R., eds., RSC publishing in Comprehensive Series in Photochemical & Photobiological Sciences, 2022, Chapter 9, pp. 197-226.
- 118) M. Pollum; L. Martínez-Fernández;<sup>1</sup> C. E. Crespo-Hernández,<sup>\*</sup> "Photochemistry of Nucleic Acid Bases and their Thio- and Aza-Analogues in Solution" (*Invited Review Chapter*), In *Topics in Current Chemistry:*

Photoinduced Phenomena in Nucleic Acids I. Nucleobases in the Gas Phase and in Solvents; Barbatti, M.; Borin, A. C.; Ullrich, S., eds., Springer-Verlag, Berlin, **2015**, 355, 245-327.

<sup>1</sup> Participated as visiting graduate student from the Autonomous University of Madrid, Spain.

- 119) R. A. Vogt; S. Rahman;<sup>†</sup> C. E. Crespo-Hernández,<sup>\*</sup> "Structure-Activity Relationships in Nitro-Aromatic Compounds" (*Invited Review Chapter*), In Practical Aspects of Computational Chemistry. Methods, Concepts and Applications; Leszczynski, J.; Shukla, M. K., eds., Springer, Netherlands, **2009**, pp. 217-240.
- 120) B. Cohen; C. E. Crespo-Hernández; P. M. Hare; B. Kohler,\* "Ultrafast Excited-State Dynamics in DNA and RNA Polymers", In *Femtochemistry and Femtobiology: Ultrafast Events in Molecular Science*; Martin, M.; Hynes, J. T.; Elsevier: Amsterdam, **2004**, p. 463-470.

### **Conference Proceedings**

121) C. E. Crespo-Hernández;\* C. N. J. Marai,<sup>†</sup> "Vertical Singlet Excitations on Adenine Dimer: A Time Dependent Density Functional Study", *AIP Conference Proceedings*, **2007**, 963, 607-610.

### Invention Disclosure, Provisional Patents, & Patents

- 1) C. E. Crespo-Hernández;\* M. Pollum, "Thiobase Compounds for Photodynamic Therapy", **2020**, USA Patent, Appl. # 16573682.
- 2) C. E. Crespo-Hernández;\* M. Pollum, "2,4-Dithiothymine, 2,4-Dithiouracil and their Mono-Substituted Derivatives as Potent Deep-Tissue UVA Chemotherapeutic Agents", **2015**, *Provisional Patent*, i.d. # 62/105,949.

### Invited Oral Presentations (May, 2006 - present)

- Development of Biocompatible Light-Activated Small Organic Molecules for Applications in Cancer Treatment and Cell Bioimaging, Heart, Lung and Blood Summer Research Program, School of Medicine, Case Western Reserve University, Cleveland, Ohio, June 26, 2025.
- Development of Biocompatible Light-Activated Small Organic Molecules for Applications in Cancer Treatment and Cell Bioimaging, Cancer Drug Discovery and Resistance Group, Case Comprehensive Cancer Center, School of Medicine, Case Western Reserve University, Cleveland, Ohio, May 20, 2025.
- 3) Biocompatible Organic Photosensitizers for Application in Cancer Treatment, Department of Chemistry, Kent State University, Kent, Ohio, September 19, 2024.
- Development of Organic Photo-Drugs for the Treatment of Cancers, 18<sup>th</sup> International Congress on Photobiology, IUPB-MEPSA World Congress, Pan Pacific, Perth, Western Australia, August 25 to 30, 2024.
- 5) Biocompatible Organic Photosensitizers for Cancer Treatment, 42<sup>nd</sup> Biennial American Society for Photobiology Meeting, Chicago, Illinois, July 27 to 30, 2024.
- 6) Sulfur-Substituted Compounds for Photodynamic Therapy, Heart, Lung and Blood Summer Research Program, School of Medicine, Case Western Reserve University, Cleveland, Ohio, July 11, 2024.
- 7) Thionated Compounds for Photodynamic Therapy, 2024 Inter-American Photochemical Society Meeting, Miramar Beach, Florida, January 3 to 6, 2024.
- 8) A Photochemical Perspective on the Molecular Origins of Life on Earth, Harvard Origins of Life Initiative, Harvard University, Cambridge, Massachusetts, December 13, 2023.
- 9) Development of Photosensitizers for the Treatment of Cancer Cells under Hypoxic Conditions, XV ELAFOT & 1st

LatASP Meeting, Maresias Beach, Brazil, October 23-26, 2023.

- Photochemistry of Sulfur-Substituted Nucleic Acids and Other Organic Compounds for Application in Photodynamic Therapy of Cancers, Light as Reagent and Product: Saturday Seminar Series, Department of Chemistry, University of Miami, WWW, October 14, 2023.
- 11) No Oxygen, No Problem! Development of Photosensitizers for the Treatment of Cancer Cells under Anoxic Conditions, Heart, Lung and Blood Summer Program, School of Medicine, Case Western Reserve University, Cleveland, Ohio, July 6, 2023.
- 12) No Oxygen, No Problem! Development of Photosensitizers for the Treatment of Cancer Cells under Anoxic Conditions, American Society for Photobiology Webinar Series, WWW, June 1, 2023.
- 13) Career Paths as an Underrepresented Faculty in STEM, Charles F. Brush High School Visit Day, Department of Chemistry, Case Western Reserve University, Cleveland, Ohio, March 7, 2023.
- 14) DNA + Light: From Chemical Origins of Life to Modifications that Enable Treatment of Cancer Cells, Chemistry Intensive for High School Students, Hawken, Gries Center, Cleveland, Ohio, December 8, 2022.
- Development and Spectroscopy Investigations of Biocompatible Photosensitizers for the Treatment of Cancer Cells, Bioinspiration for Energy Transport at the Quantum Scale (Workshop), Marseille, France, November 2 to 4, 2022.
- 16) From Lares, Puerto Rico to Cleveland, Ohio: Using DNA and Light to Promote Diversity, Equity, and Inclusion, Southeastern Regional Meeting of the American Chemical Society, The Puerto Rico Convention Center, San Juan, Puerto Rico, October 19-22, 2022.
- Development of Biocompatible Organic Photosensitizers for the Treatment of Cancer Cells, Department of Chemistry All-Alumni Reunion, Chemistry Mini-Symposium, Case Western Reserve University, Cleveland, Ohio, October 6 to 7, 2022.
- Development of All-Organic Photosensitizers for the Treatment of Cancer Cells Independent of the Oxygenation Status, 41<sup>st</sup> Biennial American Society for Photobiology Meeting, Albuquerque, New Mexico, September 25 to 28, 2022.
- 19) Using Light to Drive Therapeutic and Structural-Biology Applications, Heart, Lung and Blood Summer Program, School of Medicine, Case Western Reserve University, Cleveland, Ohio, June 15, 2022.
- 20) Development of All-Organic Photosensitizers for the Treatment of Cancer Cells Independent of the Oxygenation, Molecular Oncology (MO) Quarterly Meeting, Case CCC-MO Program, Wolstein Research Building, Case Western Reserve University, Cleveland, Ohio, May 23, 2022.
- 21) Development of All-Organic Photosensitizers for the Treatment of Cancer Cells Independent of the Oxygenation Status, 40<sup>th</sup> Puerto Rico Interdisciplinary Scientific Meeting (PRISM) and 55<sup>th</sup> American Chemical Society Junior Technical Meeting, University of Puerto Rico, Humacao Campus, Humacao, Puerto Rico, April 9, 2022.
- 22) DNA + Light: From Intrinsic Photostability of the Building Block of Life to Modifications that Enable Treatment of Skin Cancer Cells, Department of Chemistry, University of New Hampshire, Durham, New Hampshire, November 9, 2021.
- 23) DNA + Light: From Intrinsic Photostability of the Building Block of Life to Modifications that Enable Treatment of

Skin Cancer Cells, Department of Chemistry, University of Colorado, Denver, Colorado, November 5, 2021.

- 24) Recruiting Webinar: Why the Department of Chemistry at CWRU?, University of Puerto Rico at Río Piedras, Río Piedras, Puerto Rico, October 23, 2021.
- 25) DNA + Light: From Intrinsic Photostability of the DNA Bases to Modifications that Enable Treatment of Skin Cancer Cells, McNair Scholars Program, Cleveland State University, Cleveland, Ohio, September 21, 2021.
- 26) Photochemistry of Thionated Nucleobases and Detection of the Thietane Precursor in the Formation of the DNA 6-4 Photodimer, 19<sup>th</sup> Congress of the European Society for Photobiology, WWW and Salzburg, Austria, August 30 to September 3, 2021.
- 27) Heavy-Atom-Free Photosensitizers for the Treatment of Cancer Cells, 19th Congress of the European Society for Photobiology, WWW and Salzburg, Austria, August 30 to September 3, 2021.
- 28) Using Light to Drive Therapeutic and Structural-Biology Applications, Heart, Lung and Blood Summer Program, School of Medicine, Case Western Reserve University, Cleveland, Ohio, June 17, 2021.
- DNA + Light: From Intrinsic Photostability of the DNA Bases to Modifications that Enable Treatment of Skin Cancer Cells, Department of Chemistry, University of Puerto Rico at Bayamón, Bayamón, Puerto Rico, April 20, 2021.
- 30) DNA + Light: From Intrinsic Photostability of the Building Blocks of Life to Modifications that Facilitate Treatment of Skin Cancer Cells, Institute of Chemistry, University of São Paulo, São Paulo, Brazil, March 12, 2021.
- 31) DNA + Light: From Intrinsic Photostability of the DNA Bases to Modifications that Enable Treatment of Skin Cancer Cells, Department of Chemistry, Cleveland State University, Cleveland, Ohio, February 12, 2021.
- 32) Using Light to Drive Therapeutic and Structural-Biology Applications, Heart, Lung and Blood Summer Program, School of Medicine, Case Western Reserve University, Cleveland, Ohio, June 25, 2020.
- DNA + Light: From Intrinsic Photostability of Nucleic Acid Bases to Modifications that Enable Treatment of Skin Cancer Cells, Department of Chemistry, University of Puerto Rico at Mayagüez, Mayagüez, Puerto Rico, March 10, 2020.
- 34) DNA + Light: From Intrinsic Photostability of Nucleic Acid Bases to Modifications that Enable Treatment of Skin Cancer Cells, Department of Chemistry, Universidad Autónoma de Madrid, Madrid, Spain, February 10, 2020.
- 35) From Intrinsic Photostability of the Nucleic Acid Bases to Modifications that Enable Treatment of Skin Cancer Cells, Department of Chemistry and Biochemistry, University of Oregon, Eugene, Oregon, November 4, 2019.
- 36) Using Light to Drive Therapeutic and Structural-Biology Applications, Heart, Lung and Blood Summer Program, School of Medicine, Case Western Reserve University, Cleveland, Ohio, July 20, 2019.
- 37) Sunlight and the Molecular Origins of Life, Origins Seminar Series, Institute for the Science of Origins and Cleveland Museum of Natural History, Cleveland Museum of Natural History, Cleveland, Ohio, May 21, 2019.
- Photochemistry of Nucleic Acid Derivatives and Their Photodynamic Efficacy Against Human Epidermoid Carcinoma Cells, American Society for Photobiology Presidential Evening Symposia, Chicago, Illinois, May 9 to 10, 2019.

- 39) Photochemistry and Photodynamics of Heavy-Atom-Substituted Nucleobases, ACS Great Lakes Regional Meeting, Frederick Lewis Symposium, Lisle, Illinois, May 1 to 4, 2019.
- 40) DNA + Light: From Photostability of the Nucleobases to Atomic Modifications that Enable Damage to Human Epidermoid Cancer Cells, Department of Chemistry, John Carroll University, Cleveland, Ohio, March 20, 2019.
- 41) DNA + Light: From Intrinsic Photostability of Nucleic Acid Bases to Modifications that Facilitate Damage to Skin Cancer Cells, 5<sup>th</sup> Annual Targeting Excellence: Hispanic Latino Student Initiative, Department of Chemistry, University of Louisville, Louisville, Kentucky, February 22, 2019.
- 42) To Promote, or Not to Promote: DNA, Light, and other Essentials, Department of Chemistry, Case Western Reserve University, Cleveland, Ohio, September 7, 2018.
- 43) Structure-Photoreactivity Properties in Nucleic Acid Base Analogues and Their Photodynamic Efficacy Against Human Epidermoid Carcinoma Cells, Heart, Lung and Blood Summer Program, School of Medicine, Case Western Reserve University, Cleveland, Ohio, July 19, 2018.
- 44) Structure-Photoreactivity Properties in Nucleic Acid Base Analogues and Their Photodynamic Efficacy Against Human Epidermoid Carcinoma Cells, 37<sup>th</sup> Reaction Mechanisms Conference, University of British Columbia, Vancouver, Canada, June 10 to 13, 2018.
- 45) DNA + Light: From Photostability of the Nucleobases to Modifications that Enable Damage to Skin Cancer Cells, Chemistry Panel, Department of Chemistry, Case Western Reserve University, Cleveland, Ohio, March 15, 2018.
- 46) Photochemical Relaxation Pathways of S<sup>6</sup>-Methylthioinosine and O<sup>6</sup>-Methylguanosine in Solution, Photoinduced Processes in Nucleic Acids and Proteins: Faraday Discussions, Kerala, India, January 11 to 13, 2018.
- Ultrafast Intersystem Crossing in Organic Molecules without Metals, The 13<sup>th</sup> Femtochemistry Conference (FEMTO13), Frontiers of ultrafast phenomena in Chemistry, Biology, and Physics, Cancun, Mexico, August 12 to 17, 2017.
- 48) Driving Drug Development and Structural-Biology Applications using Basic (Photo)-Chemistry, Heart, Lung & Blood Summer Program, Case Western Reserve University School of Medicine, Cleveland, Ohio, July 6, 2017.
- 49) Using Fundamental Photochemistry to Drive Drug Development and Structural-Biology Applications, 253<sup>rd</sup> National American Chemical Society Meeting & Exposition, San Francisco, California, April 2 to 6, 2017.
- 50) DNA Photochemistry: From Intrinsic Photostability of the Nucleobases to Modifications that Enable Damage to Cancer Cells, Northeast by Midwest Regional Meeting (*NExM* 2017), University of Pittsburg, Pittsburgh, Pennsylvania, March 17, 2017.
- 51) DNA + Light: From Intrinsic Photostability of DNA to Modifications that Enable Damage to Cancer Cells, Department of Chemistry, The College of Wooster, Wooster, Ohio, February 28, 2017.
- 52) What Role Does Functionalization Play in the Radiative and Non-Radiative Decay Pathways in Nucleic Acid Bases?, 26th Winter Inter-American Photochemical Society Conference, Sarasota, Florida, January 2 to 5, 2017.
- 53) Photoexcitation of DNA: From Photostability of Nucleic Acids to Modifications that Enable Damage to Skin Cancer Cells, Department of Chemistry and Biochemistry, Kent State University, Kent, Ohio, October 13, 2016.

- 54) Diversity in the Physical Sciences: A Personal Journey, Multicultural Resource Center, Oberlin College, Oberlin, September 22, 2016.
- 55) DNA + Light: From Nucleic Acid Bases to Modifications that Sensitize Damage in Cells, Department of Chemistry and Biochemistry, Oberlin College, Oberlin, September 22, 2016.
- 56) Academic Career Path: How I made it?, Heart, Lung and Blood Summer Program, School of Medicine, Case Western Reserve University, Cleveland, Ohio, July 7, 2016.
- 57) From Nucleic Acid Bases to Modifications that Sensitize Damage in Cells, School of Pharmacy, East China University of Science and Technology, Shanghai, China, June 22, 2016.
- 58) From Nucleic Acid Bases to Modifications that Sensitize Damage in Cells, Department of Chemistry, East Normal University, Shanghai, China, June 21, 2016.
- 59) Kendric C. Smith Keynote Speaker: DNA + Light: From Nucleic Acid Bases to Modifications that Sensitize Damage in Cells, 38<sup>th</sup> American Society for Photobiology Meeting, Tampa, Florida, May 21 to 26, 2016.
- 60) Early Events in the Photochemistry of Nucleic Acid Bases, 47<sup>th</sup> American Chemical Society Central Regional Meeting, Covington, Northern Kentucky, Kentucky, May 18 to 21, 2016.
- 61) Diversity in the Physical Sciences: A Personal Journey, Office for Inclusion, Diversity and Equal Opportunity, Case Western Reserve University, Cleveland, Ohio, November 9, 2015.
- 62) Ultrafast Processes in DNA Photochemistry, International Symposium: Sunlight-Triggered DNA Lesions and Skin Cancer, Ramón Areces Foundation, Universitat Politècnica de València, València, Spain, November 4, 2015.
- 63) Scientific Career Path in the USA: How I make it There?, Department of Chemistry, University of Puerto Rico at Mayagüez, Mayagüez, Puerto Rico, September 18, 2015.
- 64) Electronic and Structural Elements that Regulate the Decay Pathways in Nucleic Acids, Heart, Lung and Blood Summer Program, School of Medicine, Case Western Reserve University, Cleveland, Ohio, June 11, 2015.
- 65) Electronic and Structural Elements that Regulate the Decay Pathways in Nucleic Acids, Center for Proteomics and Bioinformatics, School of Medicine, Case Western Reserve University, Cleveland, Ohio, April 16, 2015.
- 66) Invited panelist in a Faculty Panel on 'To Tenure and Beyond: Building an Intentional Career at CWRU', Office of Faculty Development, Case Western Reserve University, Cleveland, Ohio, January 27, 2015.
- 67) DNA under Attack: Electronic and Structural Elements that Regulate Nucleic Acids Photostability, 45<sup>th</sup> American Chemical Society Central Regional Meeting, Diversity in Chemical Sciences, Green Tree, Pittsburgh, PA, October 29 to November 1, 2014.
- 68) DNA under Attack: How UV Radiation Affects the Integrity of DNA, Department of Chemistry, University of Puerto Rico at Humacao, Humacao, Puerto Rico, April 22, 2014.
- 69) Ultrafast Intersystem Crossing Dynamics in Organogold(I) Aromatic Compounds, Focused-Meeting on Spin-Effects on the Ultrafast Dynamics of Photoactive Transition Metal Complexes, University of Vienna, Vienna, Austria, November 18 to 19, 2013.

- 70) DNA under Attack: How UV Radiation Affects the Integrity of DNA, Department of Chemistry, University of Louisville, Louisville, Kentucky, November 15, 2013.
- 71) DNA under Attack: How UV Radiation Affects the Integrity of DNA, Department of Chemistry, Bowling and Green State University, Bowling and Green, Ohio, October 15, 2013.
- 72) DNA under Attack: How UV Radiation Affects the Integrity of DNA, Department of Chemistry, Case Western Reserve University, Cleveland, Ohio, September 12, 2013.
- 73) Excited-State Dynamics in Sulfur-Substituted DNA Base Analogues, Gordon Research Conference on Photochemistry, Stonehill College, Easton, Massachusetts, July 14 to 19, 2013.
- 74) Participated as an invited panelist in a Faculty Panel on How to Write Successful NSF CAREER Proposals, organized by the Office of the Dean, College of Arts and Sciences, Case Western Reserve University, Cleveland, Ohio, May 15, 2013.
- 75) Academy as a Professional Career Path for Underrepresented Groups in Sciences, Minority Graduate Student Organization, School of Medicine, Case Western Reserve University, Cleveland, Ohio, April 19, 2013.
- 76) DNA under Attack: How UV Radiation Affects the Integrity of DNA, Department of Chemistry, Rice University, Houston, Texas, April 3, 2013.
- 77) The Roadway to Academia, Research Initiative for Scientific Enhancement, Biomedical Research Training Center, University of Puerto Rico, Río Piedras Campus, Puerto Rico, February 7, 2013.
- 78) DNA Photostability, DNA Photodamage: The How, the Why, and the Where, Biomedical Research Training Center, University of Puerto Rico, Río Piedras Campus, Puerto Rico, February 8, 2013.
- 79) Excited-State Dynamics in Nucleic Acids Analogues, Astrobiology Science Conference 2012, Atlanta, Georgia, April 16 to 20, 2012.
- 80) Does DNA Dynamics Come in Singlet and Triplet Flavors?, Department of Chemistry, Jackson State University, Jackson, Mississippi, October 8, 2010.
- 81) Time-Resolved Photochemistry of DNA, Department of Chemistry, University of Akron, September 14, 2010.
- 82) Shining Light on the Molecule of Life, 35<sup>th</sup> American Society for Photobiology Meeting, Providence, Rhode Island, June 12 to 16, 2010.
- Shining Light on the Molecule of Life, Department of Chemistry, Calvin College, Grand Rapids, Michigan, March 4, 2010.
- 84) Shining Light on the Molecule of Life, Department of Chemistry, Hope College, Holland, Michigan, March 5, 2010.
- Time-Resolved Photochemistry of DNA, NIH/NHLBIT35 Program, School of Medicine, Case Western Reserve University, Cleveland, Ohio, June 10, 2009.
- Ultrafast Dynamics of Biomolecules and Nitro-Aromatic Compounds, Department of Chemistry, Jackson State University, Jackson, Mississippi, March 27, 2009.

- 87) DNA Photodynamics: From Single Bases to the Double Helix, Department of Biochemistry, School of Medicine, Case Western Reserve University, Cleveland, Ohio, October 30, 2008.
- 88) Probing DNA Electronic Energy Flow and Its Mutagenic Consequences, Department of Chemistry, Cleveland State University, Cleveland, Ohio, October 10, 2008.
- 89) Academy as a Professional Career Path for Underrepresented Groups in Sciences, T35 Minority Training Grant, School of Medicine, Case Western Reserve University, Cleveland, Ohio, June 11, 2008.
- 90) Excess Energy Flow in DNA: Bench and Computer Experiments Working in Unison, Software Applications and Codes Meeting for the Ohio Supercomputer Center Bioscience Cluster Expansion, Ohio Supercomputer Center, Columbus, Ohio, April 4, 2008.
- 91) Academy as a Professional Career Path, Minority Graduate Student Organization, School of Medicine, Case Western Reserve University, Cleveland, Ohio, January 18, 2008.
- 92) Vertical Singlet Excitations on Adenine Dimer: A Time Dependent Density Functional Study, at the "Modeling Complex Molecular and Biomaterial Systems" ICCMSE Symposium, the International Conference of Computational Methods in Sciences and Engineering, Corfu, Greece, September 27 to 30, 2007.
- 93) Excited State Dynamics in Single and Double-Stranded DNA Constructs: Ultrafast Formation of the Major Radiation Product in DNA, at "Frontiers in Optics 2007", the 91<sup>st</sup> Annual Optical Society of America Meeting, San Jose, California, September 16 to 20, 2007.
- 94) Relaxation of Excess Electronic Energy and Ultrafast Formation of Thymine-Thymine Photodimer in DNA, Department of Chemistry, Case Western Reserve University, Cleveland, Ohio, January 30, 2007.
- 95) Excited State Dynamics in Nucleic Acid Monomers and Polymers: UV-Induced Ultrafast Formation of Thymine-Thymine Photodimer in DNA, Department of Chemistry, University of Houston, Houston, Texas, January 11, 2007.
- 96) Ultrafast Excited State Dynamics: Direct Observation of DNA Damage by UV Light; Department of Chemistry, University of Miami, Coral Gables, Miami, January 4, 2007.
- 97) Ultrafast Energy Relaxation in Biomolecules: Real Time Observation of DNA Damage by UV Light; Department of Chemistry, University of North Carolina, Chapel Hills, North Carolina, December 18, 2006.
- 98) From Femtochemistry to Femtobiology: Direct Observation of Excited State Dynamics and DNA Damage by UV Light; Department of Chemistry, University of Kansas, Kansas City, Kansas, December 14, 2006.
- 99) Early Events in DNA Photophysics; 17<sup>th</sup> Inter-American Photochemical Society Conference on Photochemistry, Salvador, Bahía, Brazil, June 11 to 16, 2006.
- 100) Real Time Observation of DNA Damage by Ultraviolet Radiation: New Insights Half a Century After Watson-Crick's Discovery of Double Stranded DNA; Department of Chemistry, University of Puerto Rico, San Juan Campus, San Juan, Puerto Rico, May 16, 2006.

### Contributed Oral Presentations (May, 2003 - present)

1) Subpicosecond Intersystem Crossing and Near Unity Triplet Yield I Sulfur-Substituted DNA Base Analogues upon UVA Excitation: Are these Compounds Ideal Singlet Oxygen Generators?, 5th Ohio Photochemical Society

Meeting, Oregon, Ohio, May 14 to 16, 2014.

- 2) DNA under Attack: How UV Radiation Affects the Integrity of DNA, Department of Chemistry, University of Puerto Rico at Humacao, Humacao, Puerto Rico, April 22, 2014.
- 3) UVA-Induced Dynamics in Sulfur-Substituted Nucleosides, 36<sup>th</sup> American Society for Photobiology Meeting, Montreal, Canada, June 23 to 27, 2012.
- 4) Solvent Relaxation Following Vibrational Cooling in the Triplet Manifold of 1-Nitronaphthalene, XXIV International Conference on Photochemistry, Toledo, Spain, July 19 to 24, 2009.
- 5) Base Stacking, not Base Pairing, Governs Excited-State Dynamics in A·T-Containing DNA, The 230<sup>th</sup> ACS National Meeting, Washington, DC, August 28 to September 1, 2005.
- Base Stacking, not Base Pairing, Governs Excited-State Dynamics in A·T-Containing DNA, 60<sup>th</sup> Annual Molecular Spectroscopy Symposium, Mini-symposium, Bio-relevant Molecules, Columbus, OH, June 20 to 24, 2005.
- 7) Intra- versus Inter-Strand Excited-State Dynamics in A·T-Containing Double Stranded DNA, 4<sup>th</sup> Meeting of the Ohio Photochemical Society, Oxford, Ohio, May 20 to 22, 2005.
- 8) Research in Kohler's Group, Autumn Research Presentation to First Year Graduate Students, Department of Chemistry, The Ohio State University, October 14, 2004.
- 9) *Ab initio* Ionization Energy Thresholds of DNA and RNA Bases in Gas Phase and in Aqueous Solution, 4<sup>th</sup> Southern School on Computational Chemistry, Orange Beach, Alabama, March 26 to 27, 2004.
- Photophysics of DNA and RNA Polymers Studied by Femtosecond Pump-Probe Spectroscopy, The 31<sup>st</sup> Annual Meeting of the American Society for Photobiology, Baltimore, Maryland, USA, July 5 to 9, 2003.
- 11) Photophysics of DNA and RNA Polymers Studied by Femtosecond Pump-Probe Spectroscopy, The 2<sup>nd</sup> Ohio Photochemical Society Meeting, Ohio, USA, May 16 to 18, 2003.

Published Abstracts (oral (O) and poster (P) presentations) (July, 2007 - present)

- Díaz-González, K.; Seth, S. K.; C. E. Crespo-Hernández, "Photophysical Characterization of 3-N-methyl-5-(thiophen-2-yl)-6-azauridine: A Fluorescent Nucleobase Derivate for Imaging-Assisted Photodynamic Therapy" American Chemical Society Meeting in Miniature, Case Western Reserve University, Cleveland, March 12, 2025. (O)
- C. Reyes,<sup>†</sup> R. Mathew, E. Mao, C. E. Crespo-Hernández, "Investigating The Electronic Relaxation Mechanism in Thiophene Derivatives" Intersections: Undergraduate Research Poster Session, Case Western Reserve University, Cleveland, April 18, 2025. (P) <sup>†</sup> Participated as an undergraduate student.
- R. Mathew,\* D. Mathur, S. M. Parker, C. E. Crespo-Hernández, "Efficient and Ultrafast Resonance Energy Transfer in a dsDNA-Cy3-Cy5 Construct" American Chemical Society Cleveland Local Section Meeting in Miniature, Case Western Reserve University, Cleveland, March 12, 2025. (O)
- 4) N. V. Falcón-Cruz; R. Khan; C. Aquah; L. Levi; R. Matthew; S. K. Seth; and C. E. Crespo-Hernández, "Comparative Analysis of the Photosensitization Properties of Two Alloxazine Derivatives", 2025 American

Chemical Society Cleveland Local Section Meeting in Miniature (MiM), Cleveland, OH, March 12, 2025. (O)

- T. I. Tonny; R. Mathew; C. E. Crespo-Hernández, "Studying the Electronic Relaxation Mechanisms of Amino Substituted Pyrimidine Nucleobases to Develop Structure–Photophysical Property Relationships", 2025 American Chemical Society Cleveland Local Section Meeting in Miniature (MiM), Case Western Reserve University, Cleveland, March 12, 2025. (O)
- A. Saulnier;<sup>†</sup> T. I. Tonny; C. E. Crespo-Hernández, "Ultraviolet Photodegradation of DNA and RNA Nucleotides at 266 nm", Intersections: Undergraduate Research Poster Session, Case Western Reserve University, Cleveland, April 18, 2025. (P) <sup>†</sup> Participated as an undergraduate student.
- 7) E. Lee;<sup>†</sup> C. Acquah; C. E. Crespo-Hernández, "Electronic Relaxation Mechanism of 4-Dimethylaminophthalimide and Thio-4-dimethylaminophthalimide: A Photophysical Insight for Heavy-Atom-Free Photosensitizer Development for Cancer Cells", Intersections: Undergraduate Research Poster Session, Case Western Reserve University, Cleveland, December 6, 2024. (P) <sup>†</sup> Participated as an undergraduate student.
- S. K. Seth,\* C. E. Crespo-Hernández, "6-Azauridine Derivatives as Phototheranostic and Photodynamic Therapeutic Agents for Cancer Treatment", 42<sup>nd</sup> American Society for Photobiology Biennial Meeting, Chicago, IL, July 27-30, 2024. (**O**)

## \* Winner of best oral presentation, 2nd place in postdoc category.

- S. K. Seth, C. Acquah, L. Levi, S. Jockusch, C. E. Crespo-Hernández, "Development of 5-(5-Phenylthiophen-2yl)-6-Azauridine as a Dual Phototheranostic and Cancer Cell Inhibitory Agent", 42<sup>nd</sup> American Society for Photobiology Biennial Meeting, Chicago, IL, July 27-30, 2024. (P)
- C. Acquah;\* E. Lee;<sup>†</sup> C. E. Crespo-Hernández, "Investigation of Biocompatible Organic Photosensitizers and Development of a Low Cost 3D-Printed Irradiation System for Reproducible Photodynamic Therapy Experiments", 42<sup>nd</sup> American Society for Photobiology Biennial Meeting, Chicago, IL, July 27, 2024. (P) <sup>†</sup> Participated as an undergraduate student.

# \* Winner of one of the best graduate student oral presentation.

11) C. Acquah;\* E. Lee;<sup>†</sup> C. E. Crespo-Hernández, "Investigation of Biocompatible Organic Photosensitizers and Development of a Low Cost 3D-Printed Irradiation System for Reproducible Photodynamic Therapy Experiments", 42<sup>nd</sup> American Society for Photobiology Biennial Meeting, Chicago, IL, July 27, 2024. (O) <sup>†</sup> Participated as an undergraduate student.

### \* Winner of one of the best graduate student oral presentations.

- 12) K. V. Maldonado;<sup>†</sup> Díaz-González, K.; Seth, S. K.; C. E. Crespo-Hernández, "Effect of Tautomerization in the Photophysics of 5-(thiophen-2-yl)-6-aza Uracil", 13<sup>th</sup> Department of Chemistry and American Chemical Society Project SEED Poster Presentation, 13<sup>th</sup> Department of Chemistry and American Chemical Society Project SEED Poster Presentation, Case Western Reserve University, Cleveland, July 26, 2024. (P) <sup>†</sup> Participated as a high school student.
- 13) A. Johannessen;<sup>†</sup> R. Khan; S. K. Seth; C. E. Crespo-Hernández, "Computational Study of a Chalcogen Derivative and its Thionated Analogue", Case Western Reserve University, Gilmour Academy, Cleveland, July 26, 2024. (P) <sup>†</sup> Participated as a high school student.
- 14) C. Acquah; E. Lee;<sup>†</sup> C. E. Crespo-Hernández, "Developing Biocompatible Organic Compounds as Photodynamic

Therapy Agents for Cancer Cells", IGNITE (Expanding Horizon Initiative), Case Western Reserve University, Cleveland, October 13, 2023. (O & P) † Participated as an undergraduate student.

- S. K. Seth, C. E. Crespo-Hernández, "DNA/RNA Derivatives as Prospective Phototheranostic Agents for Skin Cancer Treatment", IGNITE (Expanding Horizon Initiative), Case Western Reserve University, Cleveland, October 13, 2023. (O & P)
- 16) Feliciano-Agustín, A. D.;<sup>†</sup> Díaz-González, K.; Seth, S. K.; C. E. Crespo-Hernández, "Computational Study of a Barbituric Acid Derivative and its Thionated Analogue", 12<sup>th</sup> Department of Chemistry and American Chemical Society Project SEED Poster Presentation, Case Western Reserve University, Cleveland, July 28, 2023. <sup>†</sup> Participated as Project SEED high school student. (P)
- 17) C. Acquah; E. Lee;<sup>†</sup> C. E. Crespo-Hernández, "Developing Biocompatible Organic Compounds as Photodynamic Therapy Agents for Cancer Cells", Case Comprehensive Cancer Center Annual Scientific Retreat, Case Western Reserve University, Cleveland, July 20, 2023. (P) <sup>†</sup> Participated as an undergraduate student.
- S. K. Seth, C. E. Crespo-Hernández, "5-(5-Phenylthiophen-2-yl)-6-Azauridine: A Prospective Phototheranostic Agent for Skin Cancer Treatment", Case Comprehensive Cancer Center Annual Scientific Retreat, Case Western Reserve University, Cleveland, July 20, 2023. (P)
- 19) C. Acquah;\* E. Lee;<sup>†</sup> C. E. Crespo-Hernández, "Developing Biocompatible Organic Compounds as Photodynamic Therapy Agents for Cancer Cells", American Chemical Society Meeting in Miniature, Baldwin Wallace University, Berea, Ohio, March 15, 2023. (O) <sup>†</sup> Participated as an undergraduate student.

### \* Winner of one of the best graduate student oral presentations.

- S. K. Seth; C. E. Crespo-Hernández, "5-(5-Phenylthiophen-2-yl)-6-Azauridine: A Potential Phototheranostic Agent for Skin Cancer Treatment", American Chemical Society Meeting in Miniature, Baldwin Wallace University, Berea, Ohio, March 15, 2023. (O)
- 21) M. Pogharian;<sup>†,\*</sup> S. Hoehn, S. Krul; C. E. Crespo-Hernández, "Is 5-Methylcitidine safe for use in mRNA vaccines?", American Chemical Society Meeting in Miniature, Baldwin Wallace University, Berea, Ohio, March 15, 2023. (O) † Participated as an undergraduate student.

### \* Winner of one of the best undergraduate student oral presentations.

- 22) E. Mao; C. Griffith; C. E. Crespo-Hernández, "Electronic Relaxation Mechanism in Benzothiophene Derivatives Predicted using Time-Dependent Density Functional Calculations", American Chemical Society Meeting in Miniature, Baldwin Wallace University, Berea, Ohio, March 15, 2023. (O)
- C. Griffith; E. Mao; C. E. Crespo-Hernández, "Photophysics Properties of Thianaphthene Derivatives in Protic and Aprotic Solvents", American Chemical Society Meeting in Miniature, Baldwin Wallace University, Berea, Ohio, March 15, 2023. (O)
- 24) S. K. Seth; C. E. Crespo-Hernández, "Developing RNA and DNA Photodynamic Therapy Agents Absorbing Two Photons in the Near-Infrared for Cancer Treatment", 2022 Case Western Reserve University Innovation Week, Two-Minute Pitch Your Poster Contest, Case Western Reserve University, Cleveland, September 16, 2022. (P)
- 25) S. J. Hoehn; C. E. Crespo-Hernández, "On the Origin of the Photofitness to Light Induced Damage of DNA/RNA and its Derivatives", 2022 Case Western Reserve University Innovation Week, Two-Minute Pitch Your Poster

Contest, Case Western Reserve University, Cleveland, September 16, 2022. (P)

26) C. Acquah;\* C. E. Crespo-Hernández, "Developing Biocompatible Organic Compounds as Photodynamic Therapy Agents for Cancer Cells", 2022 Case Western Reserve University Innovation Week, Two-Minute Pitch Your Poster Contest, Case Western Reserve University, Cleveland, September 16, 2022. (P)

# \* Winner of one of the two-minute pitch your poster contest.

- 27) C. Griffith; C. E. Crespo-Hernández, "The Photophysics of Polycyclic Aromatic Compounds", 2022 Case Western Reserve University Innovation Week, Two-Minute Pitch Your Poster Contest, Case Western Reserve University, Cleveland, September 16, 2022. (P)
- 28) O. O. Ortiz;<sup>†</sup> S. Krul; C. Acquah; S. Hoehn; C. E. Crespo-Hernández, "Photochemical Studies and Photodynamic Efficacy of Sulfur Substituted Biocompatible Compounds Against Cancer Cells", CanSUR Symposium, Case Comprehensive Cancer Center, Case Western Reserve University, Cleveland, Ohio, July 28, 2022. (O) <sup>†</sup> Participated as an undergraduate student.
- 29) K. Van Allen;<sup>†</sup> S. Krul; S. Hoehn; C. E. Crespo-Hernández, "Determining the Electronic Decay Mechanisms for Hypoxanthine and 9-Deazahypoxanthine Upon Exposure of UV/C Light by Time-Resolved Transient Absorption Spectroscopy with Attention to Solvent Effects", SOURCE Virtual Spring Intersections, Case Western Reserve University, Cleveland, Ohio, April 22, 2022. (O) <sup>†</sup> Participated as an undergraduate student.
- G. Sleyko;<sup>†</sup> C. Griffith; S. Krul; S. Hoehn; C. E. Crespo-Hernández, "A Photophysical Study of Dibenzothiophene, 4-Methyldibenzothiophene, and 4,6-Dimethyldibenzothiophene", SOURCE Virtual Spring Intersections, Case Western Reserve University, Cleveland, Ohio, April 22, 2022. (O) <sup>†</sup> Participated as an undergraduate student.
- 31) M. Pogharian;<sup>†</sup> S. J. Hoehn; S. E. Krul; C. E. Crespo-Hernández, "Effects of C5-Substitution on the Photodynamics of Uracil Derivatives:5-Aminouracil, 5-Hydroxyuracil, and 5-Hydroxymethyluracil", SOURCE Virtual Fall Intersections, Case Western Reserve University, Cleveland, Ohio, December 3, 2021. (O) <sup>†</sup> Participated as an undergraduate student.
- 32) S. E. Krul; S. J. Hoehn; C. E. Crespo-Hernández, "Electronic Relaxation Mechanism of Guanine Derivatives in Solution", 76<sup>th</sup> International Symposium on Molecular Spectroscopy, University of Illinois at Urbana-Champaign, Urbana-Champaign, Illinois, June 21 to 25, 2021. (O)
- 33) S. J. Hoehn; S. E. Krul; C. E. Crespo-Hernández, "Deliberate Functionalization and the Consequential Electronic Relaxation pathways of the Pyrimidine Chromophore", 76<sup>th</sup> International Symposium on Molecular Spectroscopy, University of Illinois at Urbana-Champaign, Urbana-Champaign, Illinois, June 21 to 25, 2021. (O)
- 34) S. J. Hoehn; S. E. Krul; C. E. Crespo-Hernández, "On the Impact of Amino and Carbonyl Functionalization on the Photostability of Canonical RNA and DNA Pyrimidine Nucleobases", ACS Great Lakes Regional Meeting, hosted by Minnesota Local Section, June 6 to 9, 2021. (O)
- 35) S. E. Krul; S. J. Hoehn; C. E. Crespo-Hernández, "Effect of Selective Atom Substitution in Guanine on the Electronic Relaxation Mechanism", ACS Great Lakes Regional Meeting, hosted by Minnesota Local Section, June 6 to 9, 2021. (O)
- 36) N. E. Caldero-Rodríguez; C. E. Crespo-Hernández, "Electronic Relaxation Pathways in Nucleic Acid Derivatives Based on Functionalization of the Purine Chromophore", Case Western Reserve University, Cleveland, Ohio, February 2021 (O).

38

- 37) C. Merrick;<sup>†</sup> S. J. Hoehn; L. A. Ortiz-Rodríguez; S. E. Krul; C. E. Crespo-Hernández, "Remarkable Sensitivity of the Prospective Photodynamic Therapy Agent 6-Selenoguanine to pH", SOURCE Virtual Fall Intersections, Case Western Reserve University, Cleveland, Ohio, December, 4, 2020. <sup>†</sup> Participated as an undergraduate student. (O)
- 38) N. Abbass;<sup>†</sup> S; L. A. Ortiz-Rodríguez; C. E. Crespo-Hernández, "Is the Fluorescence Quantum Yield of Tryptophan Independent of Excitation Wavelength?", SOURCE Virtual Fall Intersections and the Celebration of Student Writing and Research, Case Western Reserve University, Cleveland, Ohio, December 4, 2020. <sup>†</sup> Participated as an undergraduate student. (O)
- B. Klucznik;<sup>†</sup> S. J. Hoehn; S. Krul, C. Merrick, <u>C. E. Crespo-Hernández</u>, "Constitutional Isomerization in Diaminopyrimidine Modulates its Electronic Relaxation Mechanism", Research ShowCase + Fall Intersections, Case Western Reserve University, Cleveland, Ohio, July 31, 2020. <sup>†</sup> Participated as undergraduate student. (O)
- C. Merrick;<sup>†</sup> S. J. Hoehn; L. A. Ortiz-Rodríguez; <u>C. E. Crespo-Hernández</u>, "Photophysical Properties of Potential Topical Photodynamic Therapy Agent 6-Selenoguanine", Research ShowCase + Fall Intersections, Case Western Reserve University, Cleveland, Ohio, July 31, 2020. <sup>†</sup> Participated as undergraduate student. (O)
- 41) S. J. Hoehn;\* S. Krul; <u>C. E. Crespo-Hernández</u>, "The Impact of Amino and Carbonyl Functionalization on the Photostability of Canonical RNA and DNA Pyrimidine Nucleobases"; American Chemical Society Meeting in Miniature, Cuyahoga Community College Western Campus, Cleveland, Parma, Ohio, March 9, 2020. (**O**)

# \* Winner of one of the best graduate student oral presentations.

- 42) S. E. Krul; S. J. Hoehn; K. Feierabend; <u>C. E. Crespo-Hernández</u>, "Generation and Dynamics of the Guanine Radical Cation in a Guanine Quadruplex Through the Absorption of Ultraviolet Radiation", American Chemical Society Meeting in Miniature, Cuyahoga Community College, Parma, Ohio, March 9, 2020. (**O**)
- C. Griffith; S. Hoehn; C. E. Crespo-Hernández, "Photochemical Study of Dibenzothiophene in Different Solvents", American Chemical Society Meeting in Miniature, Cuyahoga Community College, Parma, Ohio, March 9, 2020. (O)
- 44) B. Walker;<sup>†</sup> L. A. Ortiz-Rodríguez; <u>C. E. Crespo-Hernández</u>, "Light-Induced Damage to Prodrugs in the Presence of DNA Nucleotides", SORCE Symposium and Poster Presentation and Research ShowCase, Case Western Reserve University, Cleveland, Ohio, August 2, 2019. <sup>†</sup> Participated as undergraduate student. (P)
- 45) Malone, R.;<sup>†</sup> L. A. Ortiz-Rodríguez; <u>C. E. Crespo-Hernández</u>, "First Generation of Sulfur-Substituted Therapeutic Agents Photoactivated by Visible Light", 10<sup>th</sup> Department of Chemistry and American Chemical Society Project SEED Poster Presentation, Case Western Reserve University, Cleveland, Ohio, August 2, 2019. † Participated as Project SEED high school student. (P)
- L. A. Ortiz-Rodríguez; <u>C. E. Crespo-Hernández</u>, "Ultrafast [2+2] Cycloaddition Reaction Upon Photoactivation in Single-Stranded DNA", American Society for Photobiology Presidential Evening Symposia, Chicago, Illinois, May 9 to 10, 2019. (**O**)
- L. A. Ortiz-Rodríguez; <u>C. E. Crespo-Hernández</u>, "Ultrafast [2+2] Cycloaddition Reaction Upon Photoactivation in Single-Stranded DNA", SORCE Symposium and Poster Presentation and Research ShowCase, Case Western Reserve University, Cleveland, Ohio, April 19, 2019. (**P**)
- 48) S. J. Hoehn; L. A. Ortiz-Rodríguez; C. E. Crespo-Hernández, "Is 6-Selenoguanine an Effective Agent for Topical

39

Photodynamic Therapy and Structural Biology Applications?", SORCE Symposium and Poster Presentation and Research ShowCase, Case Western Reserve University, Cleveland, Ohio, April 19, 2019. (P)

- 49) N. E. Caldero-Rodríguez.; <u>C. E. Crespo-Hernández</u>, "Does the Amino Group Play an Important Role in the Intrinsic Photostability of the Adenine Nucleobase?", SORCE Symposium and Poster Presentation and Research ShowCase, Case Western Reserve University, Cleveland, Ohio, April 19, 2019. (P)
- L. A. Ortiz-Rodríguez; <u>C. E. Crespo-Hernández</u>, "Ultrafast [2+2] Cycloaddition Reaction Upon Photoactivation in Single-Stranded DNA", Ultrafast Photoinduced Energy and Charge Transfer, Faraday Discussions, Ventura, California, April 8 to 10, 2019. (P)
- 51) G. Ortiz-Zayas; M. Pollum; L. A. Ortiz-Rodríguez; S. Jockusch; <u>C. E. Crespo-Hernández</u>, "Photoinduced Intramolecular Electron Transfer in the Azathioprine Prodrug", Ultrafast Photoinduced Energy and Charge Transfer, Faraday Discussions, Ventura, California, April 8 to 10, 2019. (P)
- 52) S. J. Hoehn; L. A. Ortiz-Rodríguez; <u>C. E. Crespo-Hernández</u>, "Is 6-Selenoguanine an Effective Agent for Topical Photodynamic Therapy and Structural Biology Applications?"; American Chemical Society Meeting in Miniature, John Carrol University, Cleveland, Ohio, March 13, 2019. (**O**)
- 53) R. DiScipio, <u>C. E. Crespo-Hernández</u>, "Observations by Ultrafast Transient Absorption Spectroscopy: Insight into Photoreactivity of Pterin Biomolecules", The 39<sup>th</sup> Biennial Meeting of the American Society for Photobiology, Tampa Bay, Florida, May 12 to 15, 2018. (**O**)
- 54) L. A. Ortiz-Rodríguez; B. Ashwood;<sup>†</sup> C. E. Crespo-Hernández, "Photochemical Relaxation Pathways in O<sup>6</sup>-Methylguanosine and S<sup>6</sup>-Methylthioinosine Upon Absorption of Ultraviolet-B Radiation", The 39<sup>th</sup> Biennial Meeting of the American Society for Photobiology, Tampa Bay, Florida, May 12 to 15, 2018. <sup>†</sup> Participated as undergraduate student. (O)
- 55) M. Pollum; M. Lam; S. Jockusch; <u>C. E. Crespo-Hernández</u>, "Dithionated Nucleobases as Effective Photodynamic Agents Against Human Epidermoid Carcinoma Cells", The 39<sup>th</sup> Biennial Meeting of the American Society for Photobiology, Tampa Bay, Florida, May 12 to 15, 2018. (**O**)
- 56) K. Farrell;<sup>†</sup> M. M. Brister; <u>C. E. Crespo-Hernández</u>, "Enhanced Ultrafast Intersystem Crossing Dynamics for 6-Selenoguanine Relative to 6-Thioguanine", SORCE Symposium and Poster Presentation and Research ShowCase, Case Western Reserve University, Cleveland, Ohio, April 20, 2018. <sup>†</sup> Participated as undergraduate student. (P)
- 57) R. DiScipio;\* <u>C. E. Crespo-Hernández</u>, "Ultrafast Competitive Relaxation Pathways of the Pterin Chromophore", 2<sup>nd</sup> American Society for Photobiology (ASP) Associate Online Symposium, Online, August 14-21, 2017.

\* First Prize Winner for Best Poster Quality and Presentation. (P)

- 58) D. Luong;<sup>†</sup> L. A. Ortiz-Rodríguez; G. Ortiz-Zayas; <u>C. E. Crespo-Hernández</u>, "Thermodynamic Calculations of the Driving Force for Electron Transfer between DNA Bases and Their Sulfur-Substituted Analogs", ACS Project SEED Poster Session, Case Western Reserve University, Cleveland, Ohio, August 4, 2017. <sup>†</sup> Participated as Project SEED high school student. (P)
- 59) R. DiScipio; <u>C. E. Crespo-Hernández</u>, "Ultrafast Competitive Excited-State Dynamics in Substituted Pterins", Photochemistry Gordon Research Conference, Bates College, Lewiston, ME, July 23-28, 2017. (**P**)
- 60) R. DiScipio; C. E. Crespo-Hernández, "Ultrafast Competitive Excited-State Dynamics in Substituted Pterins",

Photochemistry Gordon Research Conference Graduate Seminar, Bates College, Lewiston, ME, July 22-23, 2017. (P)

- 61) K. Farrell;<sup>†</sup> R. DiScipio; <u>C. E. Crespo-Hernández</u>, "Near-Visible Light Absorption by Folic Acid: Implications to Its Suspected Cytotoxicity", Research ShowCase + Spring Intersections, Case Western Reserve University, Cleveland, Ohio, April 21, 2017. <sup>†</sup> Participated as undergraduate student. (P)
- 62) B. Ashwood;<sup>†\*</sup> M. Pollum; S. Jockusch; <u>C. E. Crespo-Hernández</u>, "The Photophysical Impacts of Glycosylation on Sulfur-Substituted DNA Nucleobases", Research ShowCase + Spring Intersections, Case Western Reserve University, Cleveland, Ohio, April 21, 2017. <sup>†</sup> Participated as undergraduate student. (O)
  - \* Winner of the 2<sup>nd</sup> Place in Natural Sciences Oral Presentation Competition.
- 63) R. DiScipio;\* <u>C. E. Crespo-Hernández</u>, "Early Events in the Absorption of Ultraviolet Light by Pterin Biomolecules", Cleveland Section of the American Chemical Society: Meeting in Miniature, Case Western Reserve University, Cleveland, Ohio, March 13, 2017. (**O**)

\* Award for Excellence in Graduate Oral Presentation.

- 64) G. Ortiz-Zayas; M. Pollum; L. A. Ortiz-Rodríguez; <u>C. E. Crespo-Hernández</u>, "Excited-State Dynamics of Thiopurine Prodrugs 6-Mercaptopurine and Azathioprine", ACS Meeting in Miniature, Cleveland State University, Cleveland, Ohio, March 13, 2017. (**O**)
- 65) B. Ashwood;<sup>†</sup> Marvin Pollum; <u>C. E. Crespo-Hernández</u>, "Excited-State Dynamics in Sulfur-Substituted Nucleobases: Photophysical Impacts of Glycosylation" Cleveland Section of the American Chemical Society: Meeting in Miniature, Cleveland State University, Cleveland, Ohio, March 13, 2017. <sup>†</sup> Participated as undergraduate student. (O)
- 66) M. M. Brister; L. E. Piñero-Santiago; M. Morel; R. Arce; and <u>C. E. Crespo-Hernández</u>, "Time-Resolved Photochemistry of Dinitropyrene Isomers" ACS Meeting-in Miniature, Cleveland State University, Cleveland, Ohio, March 13, 2017. (**O**)
- 67) K. Farrell;<sup>†</sup> M. M. Brister; <u>C. E. Crespo-Hernández</u>, "Electronic Relaxation Mechanism of Folic Acid Upon UVA Absorption", 1<sup>st</sup> Annual Multi-Section American Chemical Society Retreat: GO-Chem, Kalahari Resorts, Sandusky, Sandusky, Ohio, February 24-26, 2017. <sup>†</sup> Participated as undergraduate student. (P)
- 68) G. Ortiz-Zayas; M. Pollum; L. A. Ortiz-Rodríguez; <u>C. E. Crespo-Hernández</u>, "Photoactivation of Thiopurine Prodrugs 6-Mercaptopurine and Azathioprine and its Implications on their Side Effects", 1<sup>st</sup> Annual Multi-Section American Chemical Society Retreat: GO-Chem, Kalahari Resorts, Sandusky, Sandusky, Ohio, February 24-26, 2017. (P)
- R. DiScipio; <u>C. E. Crespo-Hernández</u>, "Ultrafast Reactive Species Generation of Pterin Biomolecules", 1<sup>st</sup> Annual Multi-Section American Chemical Society Retreat: GO-Chem, Kalahari Resort, Sandusky, Ohio, February 24-26, 2017. (**O**)
- 70) B. Ashwood;\* M. Pollum; <u>C. E. Crespo-Hernández</u>, "Unintended Consequences of Expanding the Genetic Alphabet", Cleveland State Interdisciplinary Research Conference, Cleveland State University, Cleveland, Ohio, November 5, 2016. \* Participated as an undergraduate student. (O)
- 71) B. Ashwood;\* M. Pollum; <u>C. E. Crespo-Hernández</u>, "Photo-Induced Consequences of Expanding the Genetic Alphabet", Cleveland State Interdisciplinary Research Conference, Cleveland State University, Cleveland, Ohio,

## November 5, 2016. \* Participated as an undergraduate student. (P)

- 72) L. Ortiz-Rodríguez,\* G. Ortiz-Zayas; M. Pollum; <u>C. E. Crespo-Hernández</u>, "Are Photochemical Side Effects Induced by the Azathioprine Drug or Its Metabolites?", CWRU Intersections: Summer Poster Session, Case Western Reserve University, Cleveland, Ohio, August 4, 2016. \* **Participated as an undergraduate student**. (P)
- 73) M. M. Brister; <u>C. E. Crespo-Hernández</u>, "Investigation of Ancestral Nucleobases", Astrobiology Graduate Conference, University of Boulder Colorado, Boulder, Colorado, July 25-28, 2016. **(O)**
- 74) M. Brister; M. Pollum; <u>C. E. Crespo-Hernández</u>, "On the Stability of Promising Prebiotic RNA Nucleobases Under Ultraviolet Radiation", 2016 Astrobiology Graduate Conference, Boulder, Colorado, July 24-27, 2016. (**O**)
- 75) D. Taylor;\* R. DiScipio; <u>C. E. Crespo-Hernández</u>, "Species and Excited-State Characterization of Pterin," Project SEED Poster Session, Case Western Reserve University, Cleveland, Ohio, July 29, 2016. \* Participated as a High School Student. (P)
- 76) F. Santiago;\* M. M. Brister; <u>C. E. Crespo-Hernández</u>, "Investigation of Ancestral RNA with Computational Chemistry", Project SEED Poster Session, Case Western Reserve University, Cleveland, Ohio, July 29, 2016. \* Participated as a high school student. (P)
- 77) M. Pollum; L. Guan; S. Ahsanuddi; E. Baron; M. Lam; <u>C. E. Crespo-Hernández</u>, "DNA and RNA Analogs for Topical Photodynamic Therapy", 38<sup>th</sup> American Society for Photobiology Meeting, Tampa, Florida, May 21-26, 2016. (**O**)
- 78) M. Pollum; L. Guan; S. Ahsanuddi; E. Baron; M. Lam; <u>C. E. Crespo-Hernández</u>, "Photoactivation of Sulfur-Modified DNA and RNA Analogs Induces Cytotoxicity in Epidermoid Carcinoma Cells", 2016 Society for Investigative Dermatology 75<sup>th</sup> Annual Meeting, Scottsdale, Arizona, May 11-14, 2016. (**O**)
- 79) R. DiScipio; <u>C. E. Crespo-Hernández</u>, "Early Events in the Absorption of Ultraviolet Light by Pterin Biomolecules", Research ShowCase, Case Western Reserve University, Cleveland, Ohio, April 15, 2016. (P)
- 80) M. M. Brister; <u>C. E. Crespo-Hernández</u>, "Ancestral RNA Nucleobase Investigation", Research ShowCase, Case Western Reserve University, Cleveland, Ohio, April 15, 2016. **(P)**
- 81) B. Ashwood;\* M. Pollum; <u>C. E. Crespo-Hernández</u>, "Shining Light on the Photo-Induced Risks Associated with Expanding the Genetic Alphabet", Research ShowCASE, Case Western Reserve University, Cleveland, Ohio, April 15, 2016. \* Participated as an undergraduate student. (O)
- 82) M. Pollum; L. Guan; S. Ahsanuddi; E. Baron; M. Lam; <u>C. E. Crespo-Hernández</u>, "Developing Thiobase Antimetabolites for the Photodynamic Therapy of Skin Cancer", Research ShowCase, Case Western Reserve University, Cleveland, Ohio, April 15, 2016.
- M. Brister; M. Pollum; <u>C. E. Crespo-Hernández</u>, "On the Stability of Promising Prebiotic RNA Nucleobases Under Ultraviolet Radiation", Research ShowCase, Case Western Reserve University, Cleveland, Ohio, April 15, 2016. (P)
- 84) R. DiScipio; <u>C. E. Crespo-Hernández</u>, "Early Events in the Absorption of Ultraviolet Light by Pterin Biomolecules", Cleveland Section of the American Chemical Society: Meeting in Miniature, Case Western Reserve University, Cleveland, Ohio, March 7, 2016. (**O**)

- 85) M. M. Brister; <u>C. E. Crespo-Hernández</u>, "Photochemistry of Promising Ancestral Nucleobases" ACS Meeting-in Miniature, Case Western Reserve University, Cleveland, Ohio, March 4, 2016. **(O)**
- 86) B. Ashwood;\* M. Pollum; <u>C. E. Crespo-Hernández</u>, "Potential Light-Induced Risks Associated with Expanding the Genetic Alphabet", 251<sup>st</sup> American Chemical Society National Meeting & Exposition: PHYS Poster Session, San Diego, California, March 13-17, 2016. \* **Participated as an undergraduate student. (P)**

\* Winner of the SOURCE Travel Award, Case Western Reserve University.

- 87) B. Ashwood;\* M. Pollum; <u>C. E. Crespo-Hernández</u>, "Potential Light-Induced Risks Associated with Expanding the Genetic Alphabet", 251<sup>st</sup> American Chemical Society National Meeting & Exposition: Sci-Mix Poster Session, San Diego, California, March 13-17, 2016. \* **Participated as an undergraduate student. (P)**
- 88) B. Ashwood;\*<sup>+</sup> M. Pollum; S. Jockusch; <u>C. E. Crespo-Hernández</u>, "Transient Absorption Spectroscopy Reveals the Potential Light-Induced Risks Associated with Incorporating dNaM-d5SICS", American Chemical Society Meeting in Miniature, Case Western Reserve University, Cleveland, Ohio, March 7, 2016. \* Participated as undergraduate student. (O)

### <sup>†</sup> Winner of the first place undergraduate oral presentation in Physical Chemistry.

- M. Brister; M. Pollum; <u>C. E. Crespo-Hernández</u>, "Photochemistry of Promising Ancestral RNA Nucleobases", American Chemical Society Meeting in Miniature, Case Western Reserve University, Cleveland, Ohio, March 7, 2016. (**O**)
- 90) R. DiScipio; <u>C. E. Crespo-Hernández</u>, "Electronic Relaxation Pathways in Pterin Derivatives", American Chemical Society Meeting in Miniature, Case Western Reserve University, Cleveland, Ohio, March 7, 2016. (**O**)
- 91) K. Leary;\* <u>C. E. Crespo-Hernández</u>, "Oxidative Damage of DNA and RNA Nucleotides by the Folic Acid Degradation Product, 6-Carboxypterin, Upon UVA Exposure", CWRU Intersections SOURCE Poster Presentation, Case Western Reserve University, Cleveland, Ohio, December 4, 2015. \* Participated as an undergraduate student. (P)
- 92) B. Ashwood;\*,<sup>†</sup> C. E. Crespo-Hernández, "Potential Light-Induced Risks Associated with Expanding the Genetic Alphabet", CWRU Intersections SOURCE Poster Presentation, Case Western Reserve University, Cleveland, Ohio, December 4, 2015. † Participated as undergraduate student. (P)

#### \* Second Place in Undergraduate Poster Competition.

93) B. Ashwood;\*.<sup>†</sup> M. Pollum; S. Jockusch; <u>C. E. Crespo-Hernández</u>, "Potential Light-Induced Risks Associated with Expanding the Genetic Alphabet", 9<sup>th</sup> Annual Cleveland State Interdisciplinary Research Conference, Cleveland State University, Cleveland, Ohio, November 7, 2015. <sup>†</sup> Participated as undergraduate student. (P)

### \* First Prize Winner for Best Undergraduate Poster Competition.

- 94) L. Ortiz-Rodríguez,\* M. Pollum; S. Jockusch; <u>C. E. Crespo-Hernández</u>, "Direct Measurement of the Singlet Oxygen Quantum Yield of 6-Thioguanosine", CWRU Intersections: Summer Poster Session, Case Western Reserve University, Cleveland, Ohio, July 31, 2015. \* Participated as an undergraduate student. (P)
- 95) M. Pollum; <u>C. E. Crespo-Hernández</u>, "DNA and RNA Survival Against Harsh UV Radiation on Prebiotic Earth: Will Just Any Purine Base Do?", Astrobiology Graduate Conference 2015, Madison, Wisconsin, July 19 to 23,

2015. (**O**)

- 96) M. Pollum; <u>C. E. Crespo-Hernández</u>, "Increasing the Phototherapeutic Potential of Thiobases by Understanding the Excited-State Dynamics in Nucleic Acid Bases", Gordon Research Conference on Photochemistry, Photochemistry for the Future: New Approaches, Innovations and Applications, Easton, Massachusetts, July 19 to 24, 2015. (P)
- 97) B. Ashwood;\*,† M. Pollum; <u>C. E. Crespo-Hernández</u>, "Searching Nucleic Acid Derivatives for their Potential as Extraterrestrial Building Blocks: The Case of Sulfur-Substituted DNA and RNA Analogues", Astrobiology Graduate Conference 2015, Madison, Wisconsin, July 19 to 23, 2015. † Participated as undergraduate student. (P)

# \* First Prize Winner for Best Undergraduate Poster Competition.

- 98) M. Pollum; C. Reichardt; <u>C. E. Crespo-Hernández</u>; L. Martínez-Fernández.; I. Corral; C. Rauer; S. Mai; P. Marquetand; L. González, "Which Electronic and Structural Factors Control the Photostability of DNA and RNA Purine Nucleobases?", 70<sup>th</sup> International Symposium on Molecular Spectroscopy, University of Illinois at Urbana-Champaign, Urbana-Champaign, Illinois, June 22 to 26, 2015. (**O**)
- 99) M. Brister; <u>C. E. Crespo-Hernández</u>, "Ultrafast Dynamics in DNA and RNA Derivatives Monitored by Broadband Transient Absorption Spectroscopy", 70<sup>th</sup> International Symposium on Molecular Spectroscopy, University of Illinois at Urbana-Champaign, Urbana-Champaign, Illinois, June 22 to 26, 2015. (**O**)
- 100) R. DiScipio; G. Sauvé; <u>C. E. Crespo-Hernández</u>, "Can Femtosecond Transient Absorption Spectroscopy Predict the Potential of Small Molecules as Perspective Donors for Organic Photovoltaics?", 70<sup>th</sup> International Symposium on Molecular Spectroscopy, University of Illinois at Urbana-Champaign, Urbana-Champaign, Illinois, June 22 to 26, 2015. (**O**)
- M. Pollum;\* <u>C. E. Crespo-Hernández</u>, "DNA- and RNA-Targeting Phototherapeutics Based on Sulfur-Substituted Mimics of the Natural Nucleobases", American Society for Photobiology, Inaugural Virtual Poster Symposium, June 9, 2015. (P)

# \* First Prize Winner for Best Poster.

- 102) M. Pollum; <u>C. E. Crespo-Hernández</u>, "Advancing the Photosensitizing Ability of RNA Base Derivatives by Doubling Thionation", 6<sup>th</sup> Ohio Photochemical Society Meeting, Oregon, Ohio, May 27 to 29, 2015. (**O**)
- 103) M. Brister; <u>C. E. Crespo-Hernández</u>, "Excited-State Dynamics in the RNA Base Analogue 1-Cyclohexyluracil in Acetonitrile", 6<sup>th</sup> Ohio Photochemical Society Meeting, Oregon, Ohio, May 27 to 29, 2015. (**O**)
- 104) R. DiScipio; <u>C. E. Crespo-Hernández</u>, "Effect of Chelating Metal on Photodynamics of Azadipyrromethene Complexes", 6<sup>th</sup> Ohio Photochemical Society Meeting, Oregon, Ohio, May 27 to 29, 2015. (**O**)
- 105) N. Dunn; <u>C. E. Crespo-Hernández</u>, "Ultrafast Dynamic of 2-Thiocytosine and 2-Thiocytidine in Aqueous and Organic Solutions", 6<sup>th</sup> Ohio Photochemical Society Meeting, Oregon, Ohio, May 27 to 29, 2015. (**P**)
- B. Ashwood;<sup>†</sup> M. Pollum; <u>C. E. Crespo-Hernández</u>, "Searching Nucleic Acid Derivatives for their Potential as Extraterrestrial Building Blocks: The Case of Sulfur-Substituted DNA and RNA Analogues", 6<sup>th</sup> Ohio Photochemical Society Meeting, Oregon, Ohio, May 27 to 29, 2015. <sup>†</sup> Participated as undergraduate student. (P)

- 107) M. Pollum; <u>C. E. Crespo-Hernández</u>, "Enhancing the Phototherapeutic Potential of Sulfur-Substituted DNA and RNA Analogues", Chemistry Graduate Student Symposium, University at Buffalo, The State University of New York, Buffalo, New York, May 18 to 20, 2015. (**O**)
- 108) R. DiScipio; G. Sauvé; <u>C. E. Crespo-Hernández</u>, "Excited-State Dynamics: Auxiliary Characterization for Optimizing Small-Molecules for Organic Photovoltaics", Chemistry Graduate Student Symposium, University at Buffalo, The State University of New York, Buffalo, New York, May 18 to 20, 2015. (**O**)
- 109) M. Brister; <u>C. E. Crespo-Hernández</u>, "Nucleic Acid Derivatives' Ultrafast Dynamics utilizing Broadband Transient Absorption Spectroscopy", Chemistry Graduate Student Symposium, University at Buffalo, The State University of New York, Buffalo, New York, May 18 to 20, 2015. (**O**)
- 110) M. Pollum; <u>C. E. Crespo-Hernández</u>, "DNA and RNA Analogues for Light-Activated Cancer and Disease Treatments", Research ShowCase, Case Western Reserve University, Cleveland, Ohio, April 17, 2015. (**P**)
- B. Ashwood;<sup>†</sup> M. Pollum; S. Jockusch; <u>C. E. Crespo-Hernández</u>, "Incorporating Expanded DNA Base Chromophores in E. *coli*: Potential Risks and Prospective Phototherapeutic Applications", Research ShowCase, Case Western Reserve University, Cleveland, Ohio, April 17, 2015. <sup>†</sup> Participated as undergraduate student. (P)
- M. Brister; <u>C. E. Crespo-Hernández</u>, "Investigation of DNA and RNA Nucleic Acids Using Advanced Spectroscopy Techniques", Research ShowCase, Case Western Reserve University, Cleveland, Ohio, April 17, 2015. (P)
- 113) M. Pollum; <u>C. E. Crespo-Hernández</u>, "DNA and RNA Analogues for Light-Activated Cancer and Disease Treatments", CWRU Cancer Research Fair 2015, Colleges Against Cancer, Case Western Reserve University, Cleveland, Ohio, April 3, 2015. (**P**)
- 114) M. Pollum;\* <u>C. E. Crespo-Hernández</u>, "Enhancing the Phototherapeutic Potential of Sulfur-Substituted DNA and RNA Analogues", ACS Meeting-in Miniature, Notre Dame College, South Euclid, Ohio, March 11, 2015. (**O**)

\* Graduate Student Award Winner for Oral Presentation.

- 115) DiScipio, R.; G. Sauvé; <u>C. E. Crespo-Hernández</u>, "Unraveling the Excited-State Dynamics of Small-Molecules to Scrutinize Their Prospective Use for Organic Photovoltaics", ACS Meeting-in Miniature, Notre Dame College, South Euclid, Ohio, March 11, 2015. (**O**)
- 116) H. Jenkins;<sup>†,\*</sup> K. Leary;<sup>†,\*</sup> C. E. Crespo-Hernández, "Oxidative Damage of DNA and RNA Nucleotides by the Folic Acid Derivative, 6-Carboxypterin, Upon UVA Irradiation", CWRU Intersections SOURCE Poster Presentation, Case Western Reserve University, Cleveland, Ohio, December 10, 2014. \* Participated as an undergraduate student. (P)

### <sup>†</sup> Second Place Winner in Natural Sciences & Mathematic Poster Competition.

- 117) M. Pollum; <u>C. E. Crespo-Hernández</u>, "Unraveling the Potential of Sulfur-Substituted DNA and RNA Bases as Photosensitizers", 45<sup>th</sup> American Chemical Society Central Regional Meeting, Green Tree, Pittsburgh, PA, October 29 to November 1, 2014. (P)
- 118) N. J. Dunn; M. Pollum; S. Mai; L. Matínez-Fernández; P. Marquetand; I. Corral Pérez; L. González; <u>C. E.</u> <u>Crespo-Hernández</u>, "Sub-Picosecond Intersystem Crossing Dynamics of 2-Thiocytosine in Aqueous Buffer Solution", 45<sup>th</sup> American Chemical Society Central Regional Meeting, Green Tree, Pittsburgh, PA, October 29 to

November 1, 2014. (P)

- C. Rauer; L. Matínez-Fernández; C. Reichardt; S. Mai; I. Corral; P. Marquetand; <u>C. E. Crespo-Hernández</u>;
   L. González, "The S1 as a Doorway to Intersystem Crossing in Purine a Joint Theoretical and Experimental Study", 50th Symposium on Theoretical Chemistry, University of Vienna, Austria, September 14 to 18, 2014. (P)
- 120) L. Ortiz-Rodríguez;\* M. Pollum; N. J. Dunn; <u>C. E. Crespo-Hernández</u>, "Unraveling the Photophysics of Sulfur-Substituted Nucleobases", CWRU Intersections: Summer Poster Session, Case Western Reserve University, Cleveland, Ohio, July 31, 2014. (P)

## \* Participated as an undergraduate student. Fellow of the Case-Fisk Partnership/ACES 2014 Summer Undergraduate Research Program.

- 121) M. Pollum; <u>C. E. Crespo-Hernández</u>, "The Effect of Sulfur Substitution on the Excited-State Dynamics of DNA and RNA Base Derivatives", 69<sup>th</sup> International Symposium on Molecular Spectroscopy, University of Illinois at Urbana-Champaign, Urbana-Champaign, Illinois, June 16 to 20, 2014. (**O**)
- 122) M. Pollum;\* <u>C. E. Crespo-Hernández</u>, "Unraveling the Potential of Sulfur-Substituted DNA and RNA Bases as Photosensitizers", 37<sup>th</sup> American Society for Photobiology Meeting, San Diego, California, June 14 to 19, 2014. (**O**)

# \* Winner of the American Society for Photobiology's Frederick Urbach Memorial Student Travel Award.

- 123) M. Pollum; <u>C. E. Crespo-Hernández</u>, "Unraveling the Potential of Sulfur-Substituted DNA and RNA Bases as Photosensitizers", 5<sup>th</sup> Ohio Photochemical Society Meeting, Oregon, Ohio, May 14 to 16, 2014. (**O**)
- 124) M. Brister; <u>C. E. Crespo-Hernández</u>, "Reassessment of the Ultrafast Excited-State Dynamics of 1-Cyclohexyluracil using Broadband Transient Absorption Spectroscopy", 5<sup>th</sup> Ohio Photochemical Society Meeting, Oregon, Ohio, May 14 to 16, 2014. (**O**)
- 125) R. DiScipio; G. Suavé, <u>C. E. Crespo-Hernández</u>, "Photo-kinetics of Novel Photo-voltaic Bulk-heterojunction Acceptors", 5<sup>th</sup> Ohio Photochemical Society Meeting, Oregon, Ohio, May 14 to 16, 2014. (**P**)
- M. Pollum;\* <u>C. E. Crespo-Hernández</u>, "Unraveling the Potential of Sulfur-Substituted DNA and RNA Bases as Photosensitizers", Research ShowCase, Case Western Reserve University, Cleveland, Ohio, April 18, 2014. (P)

### \* First Place Winner in Natural Sciences Poster Competition.

- 127) L. Martínez-Fernández; G. Granucci, L. González; M. Persico, C. Reichardt, <u>C. E. Crespo-Hernández</u>, I. Corral, "Structural Influence on the Photochemistry of DNA Nucleobases Derivatives", European Summer School in Quantum Chemistry, Sicily, Italy, September 8 to 21, 2013. (P)
- 128) M. Pollum; <u>C. E. Crespo-Hernández</u>, "DNA-Enhanced Dye-Sensitized Solar Cells", 68<sup>th</sup> International Symposium on Molecular Spectroscopy, The Ohio State University, Columbus, Ohio, June 17 to 21, 2013. (**O**)
- 129) Huijuan Huang; R. A. Vogt, <u>C. E. Crespo-Hernández</u>, "Excited-State Dynamics in Folic Acid and 6-Carboxypterin upon UVA Excitation", 68<sup>th</sup> International Symposium on Molecular Spectroscopy, The Ohio State University, Columbus, Ohio, June 17 to 21, 2013. (**O**)
- 130) M. Pollum; A. Adhia,<sup>†</sup> C. E. Crespo-Hernández, "Enhancing Power Conversion Efficiency in Dye-Sensitized

46

Solar Cells by Adding DNA to the Mix", 44<sup>th</sup> ACS Central Regional Meeting, Mount Pleasant, Michigan, May 15-17<sup>th</sup>, 2013. <sup>†</sup> **Participated as undergraduate student**. (**O**)

- 131) V. Laos;<sup>†</sup> H. Huang, <u>C. E. Crespo-Hernández</u>, "Does Absorption of Ultraviolet-A Light by Folic Acid Lead to DNA Damage?", Intersections: SOURCE Symposium and Poster Sessions, Case Western Reserve University, Cleveland, Ohio, April 19, 2013. <sup>†</sup> Participated as undergraduate student. (P)
- 132) Huijuan Huang; R. A. Vogt; O. Isayev; <u>C. E. Crespo-Hernández</u>, "Excited-State Dynamics in Folic Acid and 6-Carboxypterin upon UVA Excitation", Research ShowCase, Case Western Reserve University, Cleveland, Ohio, April 12, 2013. (P)
- 133) M. Pollum; A. Adhia,<sup>†</sup> <u>C. E. Crespo-Hernández</u>, "Enhancing Power Conversion Efficiency in Dye-Sensitized Solar Cells by Adding DNA to the Mix", Research ShowCase, Case Western Reserve University, Cleveland, Ohio, April 12, 2013. <sup>†</sup> Participated as undergraduate student. (P)
- 134) M. Pollum; <u>C. E. Crespo-Hernández</u>, "Tuning Förster Resonance Energy Transfer (FRET) in DNA-Fluorophore Constructs", 67<sup>th</sup> International Symposium on Molecular Spectroscopy, The Ohio State University, Columbus, Ohio, June 18 to 22, 2012. (**O**)
- 135) <u>C. E. Crespo-Hernández</u>; H. Huang; R. A. Vogt; O. Isayev, "Excited-State Dynamics of Folic Acid and 6-Carboxypterin upon UVA Excitation", 36<sup>th</sup> American Society for Photobiology Meeting, Montreal, Canada, June 23 to 27, 2012. (P)
- 136) R. A. Vogt; C. Reichardt; <u>C. E. Crespo-Hernández</u>, T. G. Gray, "Ultrafast Dynamics in Nitro- and (Organophosphine)Gold(I)-Polycylic Aromatic Hydrocarbons", ACS Meeting in Miniature, Ursuline College, Pepper Pike, Ohio, March 16, 2011. (**O**)
- 137) C. Wen; C. Reichardt; <u>C. E. Crespo-Hernández</u>, "Excited-State Dynamics in 2-Aminopurine Ribonucleoside: From Femtosecond to Microsecond Time Scale", 66th International Symposium on Molecular Spectroscopy, The Ohio State University, Columbus, Ohio, June 20-24, 2011. (**O**)
- 138) R. A. Vogt; C. Reichardt; <u>C. E. Crespo-Hernández</u>, T. G. Gray, "Ultrafast Dynamics in Nitro- and (Organophosphine)Gold(I)-Polycylic Aromatic Hydrocarbons", 66th International Symposium on Molecular Spectroscopy, The Ohio State University, Columbus, Ohio, June 20-24, 2011. (**O**)
- 139) I. Olexandr; <u>C. E. Crespo-Hernández</u>; F. C. Hill, "Toward Real-Life Petascale Applications: Experience at ERDC", 242nd ACS National Meeting & Exposition, Denver, CO, August 28 to September 1, 2011. (**O**)
- 140) I. Olexandr; D. Ghosh; <u>C. E. Crespo-Hernández</u>; A. I. Krylov, "What DFT Can Tell Us About Vertical Ionization Energy of Thymine in Water?", 242nd ACS National Meeting & Exposition, Denver, CO, August 28 to September 1, 2011. (**O**)
- 141) C. Reichardt; <u>C. E. Crespo-Hernández</u>, "Sub-Picosecond Intersystem Crossing in 4-Thiothymidine, A Nucleoside Analogue of Thymidine", XXIII IUPAC Symposium on Photochemistry, Ferrara, Italy, July 11-16, 2010. (P)
- 142) C. Reichardt; <u>C. E. Crespo-Hernández</u>, "The Dark Singlet State as Doorway State of Intersystem Crossing in DNA Monomers", 65th International Symposium on Molecular Spectroscopy, The Ohio State University, Columbus, Ohio, June 21-25, 2010. (**O**)
- 143) R. A. Vogt; C. Reichardt; C. E. Crespo-Hernández, "Ultrafast Singlet-Triplet Population Dynamics in Nitro-

Aromatic Compounds", 65th International Symposium on Molecular Spectroscopy, The Ohio State University, Columbus, Ohio, June 21-25, 2010. (**O**)

- 144) R. A. Vogt; C. Reichardt; <u>C. E. Crespo-Hernández</u>, "Ultrafast Singlet-Triplet Population Dynamics in Nitro-Aromatic Compounds", 42nd Central Regional Meeting of the American Chemical Society, ACS: Dayton, Ohio, June 16-19, 2010. (**O**)
- 145) C. Reichardt; <u>C. E. Crespo-Hernández</u>, "4-Thiothymidine: A Nucleoside Analogue of Thymidine Showing Sub-Picosecond Intersystem Crossing", 42nd Central Regional Meeting of the American Chemical Society, ACS: Dayton, Ohio, June 16-19, 2010. (**O**)
- 146) <u>C. E. Crespo-Hernández;</u> C. Reichardt, "Shining Light on the Molecule of Life", 35th American Society for Photobiology Meting, Providence, Rhode Island, June 12-16, 2010. (P)
- 147) L. G. Dodson;<sup>\*,†</sup> <u>C. E. Crespo-Hernández</u>, "On the Interaction of the Pharmaceutical Salbutamol with Light in Water Solutions", Intersections-SOURCE Symposium & Poster Session, CWRU, April 16, 2010. \* Participated as undergraduate student. (P)

### <sup>†</sup> First Place Winner in Natural Sciences Poster Competition.

- 148) L. G. Dodson;<sup>†</sup> R. A. Vogt; J. Marks;<sup>†</sup> C. Reichardt; <u>C. E. Crespo-Hernández</u>, "On the Interaction of the Pharmaceutical Salbutamol with Light in Water Solutions", Research ShowCase, CWRU, April 15, 2010. <sup>†</sup> Participated as undergraduate student. (P)
- 149) J. Santo-Pérez; <u>C. E. Crespo-Hernández</u>; C. Reichardt; I. Feliciano-Ramos; L. Arroyo-Ramírez; C. R. Cabrera; M. A. Meador, "Properties of Isomeric Electron-Withdrawing Substituted Tetraphenylbenzodifurans for Sensor and Organic Light-Emitting Diode Applications", 239th ACS National Meeting, San Francisco, CA, March 21-25, 2010. (P)
- 150) R. A. Vogt;\* C. Reichardt; <u>C. E. Crespo-Hernández</u>, "Ultrafast Branching Dynamics in Nitronaphthalene Derivatives Upon Light Absorption", ACS Meeting-in Miniature, Cleveland State University, March 17, 2010. (**O**)

#### \* First Place Winner in Oral Presentation in the Physical Chemistry Session.

- 151) C. Reichardt; R. A. Vogt; <u>C. E. Crespo-Hernández</u>, "Solvent Effects in the Vibrational Cooling Dynamics of 1-Nitronaphthalene in the Triplet Manifold", 41st Central Regional Meeting of the American Chemical Society, ACS: Cleveland, Ohio, May 20-23, 2009. (**O**)
- 152) R. A. Vogt; C. Reichardt; <u>C. E. Crespo-Hernández</u>, "Photochemistry of Nitro-Polycyclic Aromatic Compounds in Solution", 41st Central Regional Meeting of the American Chemical Society, ACS: Cleveland, Ohio, May 20-23, 2009. (**O**)
- 153) L. G. Dodson;<sup>†</sup> <u>C. E. Crespo-Hernández</u>, "Light-Induced Degradation of the Pharmaceutical Salbutamol in Aqueous Solutions", 41st Central Regional Meeting of the American Chemical Society, ACS: Cleveland, Ohio, May 20-23, 2009. <sup>†</sup> Participated as undergraduate student. (O)
- 154) C. Reichardt; R. A. Vogt; <u>C. E. Crespo-Hernández</u>, "Sub-picosecond Intersystem Crossing and Vibrational Cooling in the Triplet Manifold of 1-Nitronaphthalene", 64th International Symposium on Molecular Spectroscopy, The Ohio State University, Columbus, Ohio, June 22-26, 2009. (**O**)
- 155) C. Reichardt; R. A. Vogt; C. E. Crespo-Hernández, "Solvent Relaxation Following Vibrational Cooling of

1-Nitronaphthalene in the Triplet Manifold", XXIV International Conference on Photochemistry, Toledo, Spain, July 19-24, 2009. (**O**)

- 156) C. Reichardt; R. A. Vogt; <u>C. E. Crespo-Hernández</u>, "Solvent Effects in the Vibrational Cooling Dynamics of 1-Nitronaphthalene in the Triplet Manifold", XXIV International Conference on Photochemistry, July 19-24, 2009. (P)
- 157) C. J. Valle Díaz;<sup>†</sup> E. F. Pino López; <u>C. E. Crespo-Hernández</u>; R. Arce-Quintero, "Photophysical Characterization of 1-Nitropyrene in Different Solvents: Experimental and Computational Studies", Annual Biomedical Research Conference for Minority Students, Orlando, FI, November 5-8, 2008. <sup>†</sup> Participated as undergraduate student. (P)
- 158) M. Morel-Espinosa; R. Arce-Quintero; <u>C. E. Crespo-Hernández</u>, "Transient Species of Dinitropyrene in Solution", Abstract of Papers, 236th ACS National Meeting, Philadelphia, PA, United States, August 17-21, 2008, AEI-003. (**O**)
- 159) C. Su; C. Middleton; B. Kohler; T. Takaya; <u>C. E. Crespo-Hernández</u>, "UV/UV Femtosecond Transient Absorption Spectroscopy of Single-Stranded Adenine Multimers", 63rd International Symposium on Molecular Spectroscopy, The Ohio State University, Columbus, Ohio, June 16-20, 2008. (**O**)
- 160) K. de La Harpe; <u>C. E. Crespo-Hernández</u>; B. Cohen; B. Kohler, "The Role of Structure and Sequence on the Dynamics of Excited Electronic States in GC-Containing Oligonucleotides", 63rd International Symposium on Molecular Spectroscopy, The Ohio State University, Columbus, Ohio, June 16-20, 2008. (**O**)
- 161) B. Kohler; T. Takaya; C. Su; <u>C. E. Crespo-Hernández</u>, "On the Nature of Long-Lived Singlet Excited States in DNA", Abstract of Papers, 234th ACS National Meeting, Boston, MA, United States, August 19-23, 2007, PHYS-690. (**O**)
- 162) K. D. de La Harpe; <u>C. E. Crespo-Hernández</u>; B. Cohen; B. Kohler, "Effect of Secondary Structure on the Electronic Excited State Dynamics of d(GC)<sub>9</sub>", Abstract of Papers, 234th ACS National Meeting, Boston, MA, United States, August 19-23, 2007, PHYS-506. (**O**)