

Carlos E. Crespo-Hernández, Ph.D.

Case Western Reserve University

Department of Chemistry

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Professional Preparation	B.S. in Chemistry 1995 University of Puerto Rico , San Juan Campus, Puerto Rico Research work with R. Arce on Photochemistry of DNA and Amino Acid Components
	Ph.D. in Physical Chemistry 2002 University of Puerto Rico , San Juan Campus, Puerto Rico Graduate work with R. Arce on Photophysical and Photochemical Studies in Nucleic Acids
	NIH Postdoctoral Fellow 2003 – 2005 The Ohio State University , Columbus, OH Research work with B. Kohler on Ultrafast Excited State Dynamics in Nucleic Acids
	Research Associate 2005 – 2006 The Ohio State University , Columbus, OH Research work with B. Kohler on Ultrafast Excited State Dynamics in Single- and Double-Stranded DNA Polymers
	Appointments
	Associate Professor 2014 – present Case Western Reserve University, Cleveland, OH
	Co-director of the Center for Chemical Dynamics 2008 – present Case Western Reserve University, Cleveland, OH
	Graduate Faculty of Civil, Environmental and Architectural Engineering 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

Honors and Awards

- 1) Invited to write a review chapter for the book "*Practical Aspects of Computational Chemistry. Methods, Concepts and Applications*"; Leszczynski, J.; Shukla, M. K., eds., Springer, Netherlands (2009).
- 2) Selected in the 40-40 Club (2010). Recognizes young Hispanic leaders in the Cleveland community.
- 3) Frank Hovorka Assistant Professor of Chemistry, Case Western Reserve University (2012 – 2015).
- 4) NSF Faculty CAREER Award (2013 – 2018).
- 5) Invited to contribute with an article to the *Photochemistry and Photobiology Science* journal, as part of a themed

- issue on the "*Interaction of UV Radiation with DNA*" (2013).
- 6) Carl Storm Underrepresented Minority Fellowship, to present a talk at the 2013 Gordon Research Conference on Photochemistry.
 - 7) Invited oral presentation as part of the *Diversity in Chemical Sciences* session presented at the 45th American Chemical Society Central Regional Meeting, Green Tree, Pittsburgh, PA; October 29 to November 1, 2014.
 - 8) Member of the American Chemical Society [Canvassing Committee for the Ahmed Zewail Award in Ultrafast Science and Technology](#) (2014 – 2016).
 - 9) Invited talk for [The Power of Diversity Lectures Series](#). Office for Inclusion, Diversity and Equal Opportunity, Case Western Reserve University (2015).
 - 10) Invited to write a review chapter for the book "*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).
 - 11) Invited talk for the *International Symposium: Sunlight-Triggered DNA Lesions and Skin Cancer*, Ramón Areces Foundation, Universitat Politècnica de València, València, Spain (2015).
 - 12) Guest Editor for a high-profile Special Issue on "[Experimental and Computational Photochemistry of Bioorganic Molecules](#)" to be published in the journal *Molecules* as part of its 20th Anniversary (2016).
 - 13) Invited to contribute with an article to the *Physical Chemistry Chemical Physics* journal, as part of a themed issue on the "*Prebiotic Chemistry and Molecular Origins of Life*" (2016).
 - 14) Selected to participate in the [Denice D. Denton Emerging Leaders Workshop](#), Madison, Wisconsin (2016).
 - 15) [2016 John S. Diekhoff Award for Distinguished Graduate Student Teaching](#), Case Western Reserve University (2016).
 - 16) Keynote Speaker of the *Kendric C. Smith Interdisciplinary Symposium in Photobiology*, 38th American Society for Photobiology Meeting, Tampa, Florida (2016).
 - 17) Chair of the American Chemical Society [Canvassing Committee for the Ahmed Zewail Award in Ultrafast Science and Technology](#) (2016 – present).

PROFESSIONAL SERVICE

Service to the University and Department

- Member of the President's Advisory Council on Minorities (2015 – present).
- Member of the Executive Committee (2016).
- Member of the NOAA-AGEP Scholar Site Committee Member (2016 – present).
- Member of the Graduate Affairs Committee (2015 – 2016).
- Member of the Chemistry Resources Committee (2014 – present).
- Chair of the Chemistry Resources Committee (2014 – 2015).
- Member of the Chemistry Visibility Committee (2011 – 2015).
- Member of the Chemistry Executive Committee (2007 – 2008; 2013 – 2014).
- 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; 2017 – present).
- Member of the Energy and Material Science New Faculty Recruiting Committee (Spring 2008).
- Member of the Chemistry Resources Committee (2008 – 2011).
- 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.
- Reviewer for the CWRU Support of Undergraduate Research & Creative Endeavors (SOURCE) Program (2008 – present).
- Advisory Board Member of the Support of Undergraduate Research & Creative Endeavors at CWRU (2009 – present).
- Member of the Alpha Chi Sigma Chemistry Student Fraternity (2010 – present).

- PI 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).
- Represented the Chemistry Department in the 2011 Annual Biomedical Research Conference for Minority Students (ABRCMS) on November 9 – 12 in St. Louis, MO, in order to promote the Department and to recruit underrepresented students to our graduate program.
- 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.
- Traveled to Puerto Rico for a week to visit four campuses of the University of Puerto Rico (Cayey, Humacao, San Juan, and Mayagüez) in order 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 (November 2012).
- Traveled to University of Puerto Rico, San Juan Campus to describe undergraduate summer research opportunities in our department and to recruit students into our graduate program (February 2013).
- Traveled to Puerto Rico for a week to visit three campuses of the University of Puerto Rico (Humacao, San Juan, and Mayagüez) in order 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 (October 2014).
- Member of the College of Arts & Sciences Task Force on Research (2014 – present).
- Faculty Mentor of two Latino undergraduate students for the '*Más Allá de lo Posible*' Mentoring Program at CWRU (2014 – 2015).
- Traveled to Puerto Rico for a week to visit three campuses of the University of Puerto Rico (Humacao, San Juan, and Mayagüez) in order 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 (October 2015).
- Traveled to Puerto Rico for a week to visit three campuses of the University of Puerto Rico (Humacao, San Juan, and Mayagüez) in order 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 (October 2016).

Workshops Organized

- Many Faces of STEM (Fall 2008). A workshop and hands-on experience for underrepresented 8th and 9th graders in the Cleveland Municipal School District focusing on science, technology, engineering, and mathematics (STEM) fields.
- 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 8th and 9th graders in the Cleveland Municipal School District focusing on science, technology, engineering, and mathematics (STEM) fields.
- Preparing and Delivering Scientific Talks (Fall 2011 & 2012). Given as part of the Graduate Chemistry Retreat a seminar for 4th-year graduate students about tips for preparing and delivering scientific talks and how to effectively use visual aids.

Service to the Outside Scientific and Engineering Community

- American Society for Photobiology Engagement and Outreach Committee Member, Liaison for Latin America (2016 – 2020)
- Elected Member of the Council for the American Society for Photobiology (2016 – 2020)
- Committee Member of Grants and Awards for the American Society for Photobiology (2011 – 2015).
- Chair of the American Chemical Society Canvassing Committee for the Ahmed Zewail Award in Ultrafast Science and Technology (2016 – present).

- 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*, *Physical Chemistry Chemical Physics*, *Photochemistry and Photobiology*, *Proceedings of the National Academy of Sciences*, *Radiation Research*, and *Spectrochimica Acta* among others.
- Active reviewer of proposals for the (1) National Science Foundation, including NSF-MRI, NSF-CRIF-MU, NSF-CMI, and NSF-FCAREER review panels; (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; (7) Puerto Rico Science, Technology and Research Trust review panels.

Conferences Organized

- Symposium Chair: The 33rd American Society for Photobiology Meeting, Río Grande, Puerto Rico. Symposium: Early Events in Photochemistry and Photobiology: Section I. Ultrafast Excited State Dynamics and Charge Transfer in DNA and Section II. Fast Processes in DNA Photorepair, DNA Interactions, and Proteins. July 2006.
- Co-chair of the Physical Chemistry General Sessions: 2009 Central Regional Meeting of the American Chemical Society (CERMACS09). May 20-23, 2009.
- Symposium Co-chair: Astrobiology Science Conference 2012, Atlanta, Georgia, April 16-20, 2012.
- Organizer: The Seventy-Third Frontiers in Chemistry Series on Biophotonics, Case Western Reserve University, Department of Chemistry, Spring 2014.
- Symposium Chair: The 38th American Society for Photobiology Meeting, Tampa, Florida. Symposium: Current Topics in Photobiology, II. May 21-26, 2016.

TEACHING / MENTORING

Courses Taught

- CHEM 332: Laboratory Methods in Physical Chemistry, Spring 2008, 2009, 2010, 2011, & 2017, 3 credit hours.
- CHEM 305: Introduction to Laboratory Methods in Physical Chemistry, Spring 2009, 2010, 2011, & 2017, 3 credit hours.
- CHEM 446/337: Quantum Mechanics I, Fall 2008, 2010, 2012, & 2015, 3 credit hours.
- CHEM 406: Chemical Kinetics, Fall 2009, 2011, 2014, & 2016, 3 credit hours.
- CHEM 336: Physical Chemistry II, Spring 2012, 2013, 2014, 2015, & 2016, 3 credit hours.

Post Graduate Associates

- 1) Dr. Amy Sage (02/01/2008 – 11/30/2008).
- 2) Dr. Christian Reichardt (04/2008 – 02/28/2011)
- 3) Dr. Olexandr Isayev (04/01/2009 – 02/01/2012)

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; ongoing Ph.D.)
- 10) Regina DiScipio (start date 01/11/2013; ongoing Ph.D.)
- 11) Glesmarie Ortíz-Zayas (start date 01/11/2015; 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.
- 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) Akash Adhia (2012 – 2014) Feinberg School of Medicine, Northwestern University.
- 10) Hannah Jenkins (2011 – 2015)
- 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 – present)
- 17) Eric Jiang (2015 – 2016)
- 18) Kieran Farrell (2016 – present)
- 19) Raymond Santiago (summer 2016)
- 20) Luis Ortiz-Rodríguez (University of Puerto Rico, Humacao Campus, summer 2014, 2015 & 2016)
- 21) Michael Ward (summer 2016)

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; ACS-SEED 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 Arskanacan (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)

Recent Synergistic Activities

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

- 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 – present).
- Advisory Board Member of the Support of Undergraduate Research & Creative Endeavors at CWRU (2009 – present).
- 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.
- Many Faces of STEM, 2008 – 2011. I was actively involved in workshops for underrepresented 8th and 9th 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.
- 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).
- Program director 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.

RESEARCH / SCHOLARSHIP

Proposal and Award Activity

Current and Completed Proposals

- 1) **International Supplementary Funds (Supplementary Funds to CAREER: Mechanistic Investigations of the Excited-State Dynamics in Thiobase and Pterin UVA Sensitizers and in Their DNA Constructs)**; PI: Crespo; Source of Support: NSF; Total Award Amount: \$16,642; Total Direct Costs: \$10,600; Percent Effort: 1%; Total Award Period Covered: 6/2016–3/2018; Support: **current**.
- 2) **CAREER: Mechanistic Investigations of the Excited-State Dynamics in Thiobase and Pterin UVA Sensitizers and in Their DNA Constructs**; PI: Crespo; Source of Support: NSF CAREER; Total Award Amount: \$584,200; Total Direct Costs: \$400,736; Percent Effort: 10%; Total Award Period Covered: 4/2013–3/2018; Support: **current**.
- 3) **Research Experience for Undergraduates (Supplementary Funds to CAREER: Mechanistic Investigations of the Excited-State Dynamics in Thiobase and Pterin UVA Sensitizers and in Their DNA Constructs)**; PI: Crespo; Source of Support: NSF; Total Award Amount: \$5,748; Percent Effort: 1%; Total Award Period Covered: 6/2015–3/2018; Support: **current**.
- 4) **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: **current**.
- 5) **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: **current**.
- 6) **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: **current**.

completed.

- 7) **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**.
- 8) **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**.
- 9) **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**.
- 10) **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**.
- 11) **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**.
- 12) **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**.
- 13) **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**.
- 14) **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**.
- 15) **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**.
- 16) **Binding of DNA Components to Nitro-Compounds (Renewal)**; 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**.
- 17) **Photochemistry of Environmentally Relevant Nitro-Polycyclic Aromatic Hydrocarbons**; 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**.
- 18) **Binding of DNA Components to Nitro-Compounds (Renewal)**; 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**.
- 19) **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**.

- 20) **Binding of DNA and Amino Acids Components to Nitrogen-Rich Compounds**; 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**.
- 21) **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**.

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

- Rafael Arce, Department of Chemistry, University of Puerto Rico, San Juan, Puerto Rico, USA
- Inés Corral, Department of Chemistry, Autonomous University of Madrid, Madrid, Spain
- Leticia González, Institute for Theoretical Chemistry, University of Vienna, Vienna, Austria
- Leonid Gorb, Department of Molecular Biophysics, Institute of Molecular Biology and Genetics, National Academy of Science of Ukraine, Kyiv, Ukraine
- Thomas Gray, Department of Chemistry, Case Western Reserve University, 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
- Jerzy Leszczynski, Computational Center for Molecular Modeling Structure and Interactions, Department of Chemistry, Jackson State University, Jackson, Mississippi, USA
- Maurizio Persico, Department of Chemistry and Industrial Chemistry, University of Pisa, Pisa, Italy
- Geneviève Sauvé, Department of Chemistry, Case Western Reserve University, Cleveland, Ohio, USA
- Blanton Tolbert, Department of Chemistry, Case Western Reserve University, Cleveland, Ohio, USA
- Susanne Ullrich, Department of Physics and Astronomy, University of Georgia, Athens, Georgia, 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 is often assigned the last position.

Peer-Reviewed Publications done at CWRU (author contributions are given for collaborative work)

- 1) B. Ashwood; S. Jockusch; C. E. Crespo-Hernández. "Excited-State Dynamics of the Thiopurine Prodrug 6-Thioguanine: Can N9-Glycosylation Affects Its Phototoxic Activity?", *Molecules* **2017**, under review. **Manuscript**; submitted as part of the themed issue on the "*Experimental and Computational Photochemistry of Bioorganic Molecules*".
- 2) 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**, DOI: [10.1002/chem.201604543](https://doi.org/10.1002/chem.201604543).
- 3) 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.
- 4) 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.
- 5) B. Ashwood;† M. Pollum; C. E. Crespo-Hernández,* "Can a Six-Letter Alphabet Increase the Likelihood of

Photochemical Assault to the Genetic Code?", *Chem. Eur. J.* **2016**, *22*, 16648-16656.

† Participated as undergraduate student.

- 6) M. Pollum; B. Ashwood;† C. E. Crespo-Hernández,* "Unintended Consequences of Expanding the Genetic Alphabet", *J. Am. Chem. Soc.* **2016**, *138*, 11457-11460.

† Participated as undergraduate student.

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 [Research Highlights](#).

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](#).

- 7) M. Pollum; L. Guan; S. Ahsanuddin; E. Baron; M. Lam; C. Crespo-Hernández, "Photoactivation of sulfur-modified DNA and RNA analogs induces cytotoxicity in epidermoid carcinoma cells", *J. Invest. Dermatol.* **2016**, *136*, S105.
- 8) 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*".
- 9) 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](#).

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

† Participated as undergraduate student.

- 11) 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.
- 12) 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.

Author contributions: M.P. and C.E.C.-H. designed research; M.P. and S.J. performed research; C.E.C.-H., M.P. and S.J. analyzed data; M.P. and C.E.C.-H. wrote the paper.

- 13) 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.

Author contributions: C.E.C.-H., L.G. and I.C. designed research; L.M.-F., C.R., C.R., S.M., M.P., and P.M. performed research; C.E.C.-H., L.M.-F., C.R., C.R., S.M., M.P., L.G., and I.C. analyzed data; C.E.C.-H., L.G., I.C. wrote major parts of the paper.

- 14) 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.

Author contributions: M. P. and C.E.C.-H. designed research; M.P. and S.J. performed research; C.E.C.-H., M.P. and S.J. analyzed data; M.P. and C.E.C.-H. wrote the paper.

- 15) 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.

- 16) C. E. Crespo-Hernández;* R. A. Vogt; Sealey, B.;† "On the Primary Reaction Pathways in the Photochemistry of Nitro-Polycyclic Aromatic Hydrocarbons", *Mod. Chem. Appl.* **2013**, 1, 106 (doi: 10.4172/2329-6798.1000106).

† Fellow of the ACS Project SEED Program for economically disadvantage high school students.

- 17) 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.

- 18) Fujiwara, T.*; Reichardt, C.; Vogt, R. A.; C. E. Crespo-Hernández; Zgierski, M. Z.; Lim, E. C. "Electronic Spectra and Excited-State Dynamics of 4-Fluoro-*N,N*-dimethylaniline", *Chem. Phys. Lett.* **2013**, 586, 70-75.

Author contributions: T.F., C.E.C.-H., E.C. Lim designed research; T.F., C.R. and R.A.V. performed research; F.T. analyzed data; F.T. and C.E.C.-H. wrote the paper.

- 19) 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.

- 20) 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*".

- 21) 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.

Author contributions: C.E.C.-H. and T.G.G. designed research; R.A.V. performed research; R.A.V. and C.E.C.-H. analyzed data; and C.E.C.-H. wrote the paper.

- 22) 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.

Author contributions: O.I., C.E.C.-H., L.G., F.C.H., and J.L. designed research; O. I. performed research; O.I.

analyzed data; and O.I., C.E.C.-H., L.G., F.C.H., and J.L. wrote the paper.

- 23) 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.
- 24) L. G. Dodosn;† R. A. Vogt; J. Marks;† C. Reichardt; C. E. Crespo-Hernández,* "Photophysical and Photochemical Properties of the Pharmaceutical Compound Salbutamol in Aqueous Solutions", *Chemosphere* **2011**, 83, 1513-1523.

† Participated as undergraduate student.

- 25) 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.

Author contributions: J.S.-P., C.E.C.-H., C.R.C. and M.A.M. designed research; J.S.-P., C.E.C.-H., C.R., I.F.-R., and L.A.-R. performed research; J.S.-P., C.E.C.-H. and C.R.C. analyzed data; and J.S.-P. and C.E.C.-H. wrote the paper.

- 26) 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.

Author contributions: C.E.C.-H., A.E.A., C.G. and R.A. designed research; C.E.C.-H. and Y.D.-E. performed research; C.E.C.-H. and Y.D.-E. analyzed data; and C.E.C.-H., A.E.A.; C.G. and R.A. wrote the paper.

- 27) 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.

- 28) C. Reichardt; C. E. Crespo-Hernández,* "Ultrafast Spin Crossover in 4-Thiothymidine in an Ionic Liquid", *Chem. Commun.* **2010**, 46, 5963-5965.

- 29) 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.

Author contributions: C.E.C.-H. and T.G.G. designed research; R.A.V. and M.A.P. performed research; R.A.V. and C.E.C.-H. analyzed data; and C.E.C.-H. and T.G.G. wrote the paper.

- 30) 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).

- 31) 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.

Author contributions: D.M.C., C.E.C.-H. and L.G. designed research; D.M.C. performed research; D.M.C. and C.E.C.-H. analyzed data; J.L. contributed with computer resources; and D.M.C. and C.E.C.-H. wrote the paper.

- 32) 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.

Author contributions: C.E.C.-H. and R.A. designed research; C.E.C.-H. and B.G. performed research; C.E.C.-H.

and B.G. analyzed data; and C.E.C.-H. wrote the paper.

- 33) 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.

Author contributions: D.M.C., C.E.C.-H. and L.G. designed research; D.M.C. performed research; D.M.C. and C.E.C.-H. analyzed data; J.L. contributed with computer resources; and D.M.C. and C.E.C.-H. wrote the paper.

Other Peer-Reviewed Publications

- 1) 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.
- 2) 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*".
- 3) 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.
- 4) Y. K. Law; J. Azadi;† C. E. Crespo-Hernández; E. Olmon;† B. Kohler; "Prediction of Thymine Dimerization Yields from Molecular Dynamics Simulations", *Biophysical J.* **2008**, 94, 3590-3600. † participated as undergraduate student.
- 5) 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.
- 6) 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.
- 7) 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.
- 8) 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.
- 9) C. E. Crespo-Hernández; B. Cohen; B. Kohler,* "Molecular spectroscopy: Complexity of Excited-State Dynamics in DNA (Replay)", *Nature* **2006**, 441, E7-E8.
- 10) 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.
- 11) 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.
- 12) C. E. Crespo-Hernández; B. Cohen; B. Kohler,* "Base Stacking Controls Excited-State Dynamics in A-T-

containing DNA", *Nature* **2005**, 436, 1141-1144.

- 13) 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.
- 14) 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.
- 15) 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.
- 16) 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.
- 17) C. Crespo-Hernández; R. Arce; E. Quiñones,* "Magnetic Field Enhancement of the 6-Methylpurine Photoionization Yield", *Chem. Phys. Lett.* **2003**, 382, 661-664.
- 18) 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.
- 19) 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.
- 20) 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.
- 21) 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.
- 22) 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.
- 23) 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.
- 24) 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.

Review Articles, Book Chapters, and Conference Proceedings

Review Articles

- 1) 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.

- 2) C. E. Crespo-Hernández; B. Cohen; P. M. Hare; B. Kohler,* "Ultrafast Excited-State Dynamics in Nucleic Acids", *Chem. Rev.* **2004**, 104, 1977-2019.

Book Chapters

- 1) M. Pollum; L. Martínez-Fernández;† C. E. Crespo-Hernández,* "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.

† Participated as visiting graduate student from the Autonomous University of Madrid, Spain.

- 2) R. A. Vogt; S. Rahman;† C. E. Crespo-Hernández,* "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. † participated as undergraduate student.

- 3) 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.

Invention Disclosure, Provisional Patents, & Patents

- 1) 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.

Conference Proceedings

- 1) C. E. Crespo-Hernández;* C. N. J. Marai,† "Vertical Singlet Excitations on Adenine Dimer: A Time Dependent Density Functional Study", *AIP Conference Proceedings*, **2007**, 963, 607-610. † participated as undergraduate student.

Invited Oral Presentations (May, 2006 – present)

- 1) 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 2-5, 2017.
- 2) 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.
- 3) Diversity in the Physical Sciences: A Personal Journey, Multicultural Resource Center, Oberlin College, Oberlin, September 22, 2016.
- 4) DNA + Light: From Nucleic Acid Bases to Modifications that Sensitize Damage in Cells, Department of Chemistry and Biochemistry, Oberlin College, Oberlin, September 22, 2016.
- 5) 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.
- 6) 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.
- 7) From Nucleic Acid Bases to Modifications that Sensitize Damage in Cells, Department of Chemistry, East

Normal University, Shanghai, China, June 21, 2016.

- 8) Kendric C. Smith Keynote Speaker: DNA + Light: From Nucleic Acid Bases to Modifications that Sensitize Damage in Cells, 38th American Society for Photobiology Meeting, Tampa, Florida, May 21-26, 2016.
- 9) Early Events in the Photochemistry of Nucleic Acid Bases, 47th American Chemical Society Central Regional Meeting, Covington, Northern Kentucky, Kentucky, May 18-21, 2016.
- 10) Diversity in the Physical Sciences: A Personal Journey, Office for Inclusion, Diversity and Equal Opportunity, Case Western Reserve University, Cleveland, Ohio, November 9, 2015.
- 11) 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.
- 12) 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.
- 13) 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.
- 14) 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.
- 15) 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.
- 16) DNA under Attack: Electronic and Structural Elements that Regulate Nucleic Acids Photostability, 45th American Chemical Society Central Regional Meeting, Diversity in Chemical Sciences, Green Tree, Pittsburgh, PA, October 29 to November 1, 2014.
- 17) 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.
- 18) 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 18-19, 2013.
- 19) DNA under Attack: How UV Radiation Affects the Integrity of DNA, Department of Chemistry, University of Louisville, Louisville, Kentucky, November 15, 2013.
- 20) 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.
- 21) DNA under Attack: How UV Radiation Affects the Integrity of DNA, Department of Chemistry, Case Western Reserve University, Cleveland, Ohio, September 12, 2013.
- 22) Excited-State Dynamics in Sulfur-Substituted DNA Base Analogues, Gordon Research Conference on Photochemistry, Stonehill College, Easton, Massachusetts, July 14 to 19, 2013.
- 23) 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.

- 24) 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.
- 25) DNA under Attack: How UV Radiation Affects the Integrity of DNA, Department of Chemistry, Rice University, Houston, Texas, April 3, 2013.
- 26) 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.
- 27) 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.
- 28) Excited-State Dynamics in Nucleic Acids Analogues, Astrobiology Science Conference 2012, Atlanta, Georgia, April 16-20, 2012.
- 29) Does DNA Dynamics Come in Singlet and Triplet Flavors?, Department of Chemistry, Jackson State University, Jackson, Mississippi, October 8, 2010.
- 30) Time-Resolved Photochemistry of DNA, Department of Chemistry, University of Akron, September 14, 2010.
- 31) Shining Light on the Molecule of Life, 35th American Society for Photobiology Meeting, Providence, Rhode Island, June 12-16, 2010.
- 32) Shining Light on the Molecule of Life, Department of Chemistry, Calvin College, Grand Rapids, Michigan, March 4, 2010.
- 33) Shining Light on the Molecule of Life, Department of Chemistry, Hope College, Holland, Michigan, March 5, 2010.
- 34) Time-Resolved Photochemistry of DNA, NIH/NHLBIT35 Program, School of Medicine, Case Western Reserve University, Cleveland, Ohio, June 10, 2009.
- 35) Ultrafast Dynamics of Biomolecules and Nitro-Aromatic Compounds, Department of Chemistry, Jackson State University, Jackson, Mississippi, March 27, 2009.
- 36) DNA Photodynamics: From Single Bases to the Double Helix, Department of Biochemistry, School of Medicine, Case Western Reserve University, Cleveland, Ohio, October 30, 2008.
- 37) Probing DNA Electronic Energy Flow and Its Mutagenic Consequences, Department of Chemistry, Cleveland State University, Cleveland, Ohio, October 10, 2008.
- 38) 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.
- 39) 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.

- 40) Academy as a Professional Career Path, Minority Graduate Student Organization, School of Medicine, Case Western Reserve University, Cleveland, Ohio, January 18, 2008.
- 41) 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 27-30, 2007.
- 42) 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 91st Annual Optical Society of America Meeting, San Jose, California, September 16-20, 2007.
- 43) 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.
- 44) 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.
- 45) Ultrafast Excited State Dynamics: Direct Observation of DNA Damage by UV Light; Department of Chemistry, University of Miami, Coral Gables, Miami, January 4, 2007.
- 46) 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.
- 47) 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.
- 48) Early Events in DNA Photophysics; 17th Inter-American Photochemical Society Conference on Photochemistry, Salvador, Bahia, Brazil, June 11-June 16, 2006.
- 49) 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, 36th 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 230th ACS National Meeting, Washington, DC, August 28 – September 1, 2005.

- 6) Base stacking, not base pairing, governs excited-state dynamics in A-T-containing DNA, 60th Annual Molecular Spectroscopy Symposium, Mini-symposium, Bio-relevant Molecules, Columbus, OH, June 20-24, 2005.
- 7) Intra- versus Inter-Strand Excited-State Dynamics in A-T-Containing Double Stranded DNA, 4th Meeting of the Ohio Photochemical Society, Oxford, Ohio, May 20-22, 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, 4th Southern School on Computational Chemistry, Orange Beach, Alabama, March 26-27, 2004.
- 10) Photophysics of DNA and RNA Polymers Studied by Femtosecond Pump-Probe Spectroscopy, The 31st Annual Meeting of the American Society for Photobiology, Baltimore, Maryland, USA, July 5-9, 2003.
- 11) Photophysics of DNA and RNA Polymers Studied by Femtosecond Pump-Probe Spectroscopy, The 2nd Ohio Photochemical Society Meeting, Ohio, USA, May 16-18, 2003.

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

- 1) B. Ashwood;* M. Pollum; C. E. Crespo-Hernández, "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)**
- 2) B. Ashwood;* M. Pollum; C. E. Crespo-Hernández, "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)**
- 3) L. Ortiz-Rodríguez;* G. Ortiz-Zayas; M. Pollum; C. E. Crespo-Hernández, "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)**
- 4) M. M. Brister; C. E. Crespo-Hernández, "Investigation of Ancestral Nucleobases", Astrobiology Graduate Conference, University of Boulder Colorado, Boulder, Colorado, July 25-28, 2016. **(O)**
- 5) M. Brister; M. Pollum; C. E. Crespo-Hernández, "On the Stability of Promising Prebiotic RNA Nucleobases Under Ultraviolet Radiation", 2016 Astrobiology Graduate Conference, Boulder, Colorado, Ohio, July 24-27, 2016. **(O)**
- 6) D. Taylor*, R. DiScipio, C. E. Crespo-Hernández, "Species and Excited-State Characterization of Pterin," Project SEED Poster Session, Case Western Reserve University, July 29, 2016. * **Participated as a High School Student. (P)**
- 7) F. Santiago;* M. M. Brister; C. E. Crespo-Hernández, "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)**
- 8) M. Pollum; L. Guan; S. Ahsanuddin; E. Baron; M. Lam; C. E. Crespo-Hernández, "DNA and RNA Analogs for Topical Photodynamic Therapy", 38th American Society for Photobiology Meeting, Tampa, Florida, May 21-26, 2016. **(O)**

- 9) M. Pollum; L. Guan; S. Ahsanuddi; E. Baron; M. Lam; C. E. Crespo-Hernández, "Photoactivation of Sulfur-Modified DNA and RNA Analogs Induces Cytotoxicity in Epidermoid Carcinoma Cells", 2016 Society for Investigative Dermatology 75th Annual Meeting, Scottsdale, Arizona, May 11-14, 2016. (O)
 - 10) R. DiScipio, C. E. Crespo-Hernández, "Early Events in the Absorption of Ultraviolet Light by Pterin Biomolecules", Research ShowCase, Case Western Reserve University, Cleveland, Ohio, April 15, 2016. (P)
 - 11) M. M. Brister; C. E. Crespo-Hernández, "Ancestral RNA Nucleobase Investigation", Research ShowCase, Case Western Reserve University, Cleveland, Ohio, April 15, 2016. (P)
 - 12) B. Ashwood;* M. Pollum; C. E. Crespo-Hernández, "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)
 - 13) M. Pollum; L. Guan; S. Ahsanuddi; E. Baron; M. Lam; C. E. Crespo-Hernández, "Developing Thiobase Antimetabolites for the Photodynamic Therapy of Skin Cancer", Research ShowCase, Case Western Reserve University, Cleveland, Ohio, April 15, 2016.
 - 14) M. Brister; M. Pollum; C. E. Crespo-Hernández, "On the Stability of Promising Prebiotic RNA Nucleobases Under Ultraviolet Radiation", Research ShowCase, Case Western Reserve University, Cleveland, Ohio, April 15, 2016. (P)
 - 15) R. DiScipio, C. E. Crespo-Hernández, "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)
 - 16) M. M. Brister; C. E. Crespo-Hernández, "Photochemistry of Promising Ancestral Nucleobases" ACS Meeting-in Miniature, Case Western Reserve University, Cleveland, Ohio, March 4, 2016. (O)
 - 17) B. Ashwood;* M. Pollum; C. E. Crespo-Hernández, "Potential Light-Induced Risks Associated with Expanding the Genetic Alphabet", 251st 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.*
- 18) B. Ashwood;* M. Pollum; C. E. Crespo-Hernández, "Potential Light-Induced Risks Associated with Expanding the Genetic Alphabet", 251st American Chemical Society National Meeting & Exposition: Sci-Mix Poster Session, San Diego, California, March 13-17, 2016. * Participated as an undergraduate student. (P)
 - 19) B. Ashwood;*[†] M. Pollum; S. Jockusch; C. E. Crespo-Hernández, "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)
- [†] *Winner of the first place undergraduate oral presentation in Physical Chemistry.*
- 20) M. Brister; M. Pollum; C. E. Crespo-Hernández, "Photochemistry of Promising Ancestral RNA Nucleobases", American Chemical Society Meeting in Miniature, Case Western Reserve University, Cleveland, Ohio, March 7, 2016. (O)
 - 21) R. DiScipio; C. E. Crespo-Hernández, "Electronic Relaxation Pathways in Pterin Derivatives", American

Chemical Society Meeting in Miniature, Case Western Reserve University, Cleveland, Ohio, March 7, 2016. (O)

- 22) K. Leary; * C. E. Crespo-Hernández, "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)
- 23) B. Ashwood; *[†] 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.*
- 24) B. Ashwood; *[†] M. Pollum; S. Jockusch; C. E. Crespo-Hernández, "Potential Light-Induced Risks Associated with Expanding the Genetic Alphabet", 9th Annual Cleveland State Interdisciplinary Research Conference, Cleveland State University, Cleveland, Ohio, November 7, 2015. [†] **Participated as undergraduate student.** (P)
- * First Prize Winner for Best Undergraduate Poster Competition.*
- 25) L. Ortiz-Rodríguez; * M. Pollum; S. Jockusch; C. E. Crespo-Hernández, "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)
- 26) M. Pollum; C. E. Crespo-Hernández, "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)
- 27) M. Pollum; C. E. Crespo-Hernández, "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)
- 28) B. Ashwood; *[†] M. Pollum; C. E. Crespo-Hernández, "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.*
- 29) M. Pollum; C. Reichardt; C. E. Crespo-Hernández; 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?", 70th International Symposium on Molecular Spectroscopy, University of Illinois at Urbana-Champaign, Urbana-Champaign, Illinois, June 22 to 26, 2015. (O)
- 30) M. Brister; C. E. Crespo-Hernández, "Ultrafast Dynamics in DNA and RNA Derivatives Monitored by Broadband Transient Absorption Spectroscopy", 70th International Symposium on Molecular Spectroscopy, University of Illinois at Urbana-Champaign, Urbana-Champaign, Illinois, June 22 to 26, 2015. (O)
- 31) R. DiScipio; G. Sauvé; C. E. Crespo-Hernández, "Can Femtosecond Transient Absorption Spectroscopy Predict the Potential of Small Molecules as Perspective Donors for Organic Photovoltaics?", 70th International Symposium on Molecular Spectroscopy, University of Illinois at Urbana-Champaign, Urbana-Champaign, Illinois,

June 22 to 26, 2015. (O)

- 32) M. Pollum; * C. E. Crespo-Hernández, "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.*

- 33) M. Pollum; C. E. Crespo-Hernández, "Advancing the Photosensitizing Ability of RNA Base Derivatives by Doubling Thionation", 6th Ohio Photochemical Society Meeting, Oregon, Ohio, May 27 to 29, 2015. (O)
- 34) M. Brister; C. E. Crespo-Hernández, "Excited-State Dynamics in the RNA Base Analogue 1-Cyclohexyluracil in Acetonitrile", 6th Ohio Photochemical Society Meeting, Oregon, Ohio, May 27 to 29, 2015. (O)
- 35) R. DiScipio; C. E. Crespo-Hernández, "Effect of Chelating Metal on Photodynamics of Azadipyromethene Complexes", 6th Ohio Photochemical Society Meeting, Oregon, Ohio, May 27 to 29, 2015. (O)
- 36) N. Dunn; C. E. Crespo-Hernández, "Ultrafast Dynamic of 2-Thiocytosine and 2-Thiocytidine in Aqueous and Organic Solutions", 6th Ohio Photochemical Society Meeting, Oregon, Ohio, May 27 to 29, 2015. (P)
- 37) B. Ashwood; † M. Pollum; C. E. Crespo-Hernández, "Searching Nucleic Acid Derivatives for their Potential as Extraterrestrial Building Blocks: The Case of Sulfur-Substituted DNA and RNA Analogues", 6th Ohio Photochemical Society Meeting, Oregon, Ohio, May 27 to 29, 2015. † **Participated as undergraduate student.** (P)
- 38) M. Pollum; C. E. Crespo-Hernández, "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)
- 39) R. DiScipio; G. Sauvé; C. E. Crespo-Hernández, "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)
- 40) M. Brister; C. E. Crespo-Hernández, "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)
- 41) M. Pollum; C. E. Crespo-Hernández, "DNA and RNA Analogues for Light-Activated Cancer and Disease Treatments", Research ShowCase, Case Western Reserve University, Cleveland, Ohio, April 17, 2015. (P)
- 42) B. Ashwood; † M. Pollum; S. Jockusch; C. E. Crespo-Hernández, "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. † **Participated as undergraduate student.** (P)
- 43) M. Brister; C. E. Crespo-Hernández, "Investigation of DNA and RNA Nucleic Acids Using Advanced Spectroscopy Techniques", Research ShowCase, Case Western Reserve University, Cleveland, Ohio, April 17, 2015. (P)
- 44) M. Pollum; C. E. Crespo-Hernández, "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)

- 45) M. Pollum; * C. E. Crespo-Hernández, "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.*

- 46) DiScipio, R.; G. Sauvé; C. E. Crespo-Hernández, "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)

- 47) H. Jenkins;†* K. Leary;†* 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)

† Second Place Winner in Natural Sciences & Mathematic Poster Competition.

- 48) M. Pollum; C. E. Crespo-Hernández, "Unraveling the Potential of Sulfur-Substituted DNA and RNA Bases as Photosensitizers", 45th American Chemical Society Central Regional Meeting, Green Tree, Pittsburgh, PA, October 29 to November 1, 2014. (P)

- 49) N. J. Dunn; M. Pollum; S. Mai; L. Matínez-Fernández; P. Marquetand; I. Corral Pérez; L. González; C. E. Crespo-Hernández, "Sub-Picosecond Intersystem Crossing Dynamics of 2-Thiocytosine in Aqueous Buffer Solution", 45th American Chemical Society Central Regional Meeting, Green Tree, Pittsburgh, PA, October 29 to November 1, 2014. (P)

- 50) C. Rauer; L. Matínez-Fernández; C. Reichardt; S. Mai; I. Corral; P. Marquetand; C. E. Crespo-Hernández; 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)

- 51) L. Ortiz-Rodríguez; * M. Pollum; N. J. Dunn; C. E. Crespo-Hernández, "Unraveling the Photophysics of Sulfur-Substituted Nucleobases", CWRU Intersections: Summer Poster Session, Case Western Reserve University, Cleveland, Ohio, July 31, 2014. * **Participated as an undergraduate student. Fellow of the Case-Fisk Partnership/ACES 2014 Summer Undergraduate Research Program.** (P)

- 52) M. Pollum; C. E. Crespo-Hernández, "The Effect of Sulfur Substitution on the Excited-State Dynamics of DNA and RNA Base Derivatives", 69th International Symposium on Molecular Spectroscopy, University of Illinois at Urbana-Champaign, Urbana-Champaign, Illinois, June 16 to 20, 2014. (O)

- 53) M. Pollum; * C. E. Crespo-Hernández, "Unraveling the Potential of Sulfur-Substituted DNA and RNA Bases as Photosensitizers", 37th 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.*

- 54) M. Pollum; C. E. Crespo-Hernández, "Unraveling the Potential of Sulfur-Substituted DNA and RNA Bases as Photosensitizers", 5th Ohio Photochemical Society Meeting, Oregon, Ohio, May 14 to 16, 2014. (O)

- 55) M. Brister; C. E. Crespo-Hernández, "Reassessment of the Ultrafast Excited-State Dynamics of 1-Cyclohexyluracil using Broadband Transient Absorption Spectroscopy", 5th Ohio Photochemical Society Meeting,

Oregon, Ohio, May 14 to 16, 2014. (O)

- 56) R. DiScipio; G. Suavé, C. E. Crespo-Hernández, "Photo-kinetics of Novel Photo-voltaic Bulk-heterojunction Acceptors", 5th Ohio Photochemical Society Meeting, Oregon, Ohio, May 14 to 16, 2014. (P)
- 57) M. Pollum; * C. E. Crespo-Hernández, "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.*
- 58) L. Martínez-Fernández; G. Granucci, L. González; M. Persico, C. Reichardt, C. E. Crespo-Hernández, 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)
- 59) M. Pollum; C. E. Crespo-Hernández, "DNA-Enhanced Dye-Sensitized Solar Cells", 68th International Symposium on Molecular Spectroscopy, The Ohio State University, Columbus, Ohio, June 17 to 21, 2013. (O)
- 60) Huijuan Huang; R. A. Vogt, C. E. Crespo-Hernández, "Excited-State Dynamics in Folic Acid and 6-Carboxypterin upon UVA Excitation", 68th International Symposium on Molecular Spectroscopy, The Ohio State University, Columbus, Ohio, June 17 to 21, 2013. (O)
- 61) M. Pollum; A. Adhia,† C. E. Crespo-Hernández, "Enhancing Power Conversion Efficiency in Dye-Sensitized Solar Cells by Adding DNA to the Mix", 44th ACS Central Regional Meeting, Mount Pleasant, Michigan, May 15-17th, 2013. † Participated as undergraduate student. (O)
- 62) V. Laos;† H. Huang, C. E. Crespo-Hernández, "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. † Participated as undergraduate student. (P)
- 63) Huijuan Huang; R. A. Vogt; O. Isayev; C. E. Crespo-Hernández, "Excited-State Dynamics in Folic Acid and 6-Carboxypterin upon UVA Excitation", Research ShowCase, Case Western Reserve University, Cleveland, Ohio, April 12, 2013. (P)
- 64) M. Pollum; A. Adhia,† C. E. Crespo-Hernández, "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. † Participated as undergraduate student. (P)
- 65) M. Pollum; C. E. Crespo-Hernández, "Tuning Förster Resonance Energy Transfer (FRET) in DNA-Fluorophore Constructs", 67th International Symposium on Molecular Spectroscopy, The Ohio State University, Columbus, Ohio, June 18 to 22, 2012. (O)
- 66) C. E. Crespo-Hernández; H. Huang; R. A. Vogt; O. Isayev, "Excited-State Dynamics of Folic Acid and 6-Carboxypterin upon UVA Excitation", 36th American Society for Photobiology Meeting, Montreal, Canada, June 23 to 27, 2012. (P)
- 67) R. A. Vogt; C. Reichardt; C. E. Crespo-Hernández, T. G. Gray, "Ultrafast Dynamics in Nitro- and (Organophosphine)Gold(I)-Polycyclic Aromatic Hydrocarbons", ACS Meeting in Miniature, Ursuline College, Pepper Pike, Ohio, March 16, 2011. (O)
- 68) C. Wen; C. Reichardt; C. E. Crespo-Hernández, "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)

- 69) R. A. Vogt; C. Reichardt; C. E. Crespo-Hernández, T. G. Gray, "Ultrafast Dynamics in Nitro- and (Organophosphine)Gold(I)-Polycyclic Aromatic Hydrocarbons", 66th International Symposium on Molecular Spectroscopy, The Ohio State University, Columbus, Ohio, June 20-24, 2011. (O)
- 70) I. Olexandr; C. E. Crespo-Hernández; 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)
- 71) I. Olexandr; D. Ghosh; C. E. Crespo-Hernández; 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)
- 72) C. Reichardt; C. E. Crespo-Hernández, "Sub-Picosecond Intersystem Crossing in 4-Thiothymidine, A Nucleoside Analogue of Thymidine", XXIII IUPAC Symposium on Photochemistry, Ferrara, Italy, July 11-16, 2010. (P)
- 73) C. Reichardt; C. E. Crespo-Hernández, "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)
- 74) 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)
- 75) R. A. Vogt; C. Reichardt; C. E. Crespo-Hernández, "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)
- 76) C. Reichardt; C. E. Crespo-Hernández, "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)
- 77) C. E. Crespo-Hernández; C. Reichardt, "Shining Light on the Molecule of Life", 35th American Society for Photobiology Meeting, Providence, Rhode Island, June 12-16, 2010. (P)
- 78) L. G. Dodson;*† C. E. Crespo-Hernández, "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)
- † *First Place Winner in Natural Sciences Poster Competition.*
- 79) L. G. Dodson;† R. A. Vogt; J. Marks;† C. Reichardt; C. E. Crespo-Hernández, "On the Interaction of the Pharmaceutical Salbutamol with Light in Water Solutions", Research ShowCase, CWRU, April 15, 2010. † **Participated as undergraduate student.** (P)
- 80) J. Santo-Pérez; C. E. Crespo-Hernández; 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)
- 81) R. A. Vogt;* C. Reichardt; C. E. Crespo-Hernández, "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.*

- 82) C. Reichardt; R. A. Vogt; C. E. Crespo-Hernández, "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)
- 83) R. A. Vogt; C. Reichardt; C. E. Crespo-Hernández, "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)
- 84) L. G. Dodson;† C. E. Crespo-Hernández, "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. † **Participated as undergraduate student.** (O)
- 85) C. Reichardt; R. A. Vogt; C. E. Crespo-Hernández, "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)
- 86) 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)
- 87) C. Reichardt; R. A. Vogt; C. E. Crespo-Hernández, "Solvent Effects in the Vibrational Cooling Dynamics of 1-Nitronaphthalene in the Triplet Manifold", XXIV International Conference on Photochemistry, July 19-24, 2009. (P)
- 88) C. J. Valle Díaz;† E. F. Pino López; C. E. Crespo-Hernández; R. Arce-Quintero, "Photophysical Characterization of 1-Nitropyrene in Different Solvents: Experimental and Computational Studies", Annual Biomedical Research Conference for Minority Students, Orlando, FL, November 5-8, 2008. † **Participated as undergraduate student.** (P)
- 89) M. Morel-Espinosa; R. Arce-Quintero; C. E. Crespo-Hernández, "Transient Species of Dinitropyrene in Solution", Abstract of Papers, 236th ACS National Meeting, Philadelphia, PA, United States, August 17-21, 2008, AEI-003. (O)
- 90) C. Su; C. Middleton; B. Kohler; T. Takaya; C. E. Crespo-Hernández, "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)
- 91) K. de La Harpe; C. E. Crespo-Hernández; 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)
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