

**Carlos E. Crespo-Hernández, Ph.D.**

**Case Western Reserve University**

**Department of Chemistry**

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<b>Professional Preparation</b>	<b>B.S. in Chemistry</b>	1995
	<b>University of Puerto Rico</b> , San Juan Campus, Puerto Rico Research work with R. Arce on Photochemistry of DNA and Amino Acid Components	
	<b>Ph.D. in Physical Chemistry</b>	2002
	<b>University of Puerto Rico</b> , San Juan Campus, Puerto Rico Graduate work with R. Arce on Photophysical and Photochemical Studies in Nucleic Acids	
	<b>NIH Postdoctoral Fellow</b>	2003 – 2005
	<b>The Ohio State University</b> , Columbus, OH Research work with B. Kohler on Ultrafast Excited State Dynamics in Nucleic Acids	
	<b>Research Associate</b>	2005 – 2006
	<b>The Ohio State University</b> , Columbus, OH Research work with B. Kohler on Ultrafast Excited State Dynamics in Single- and Double-Stranded DNA Polymers	
<b>Appointments</b>	<b>Assistant Professor</b>	2007 – present
	Case Western Reserve University, Cleveland, OH	
	<b>Co-director of the Center for Chemical Dynamics</b>	2008 – present
	Case Western Reserve University, Cleveland, OH	
	<b>Editorial Member of the journal ISRN Spectroscopy</b>	2011 – present
	<b>Committee Member of Grants and Awards for the American Society for Photobiology</b>	2011 – present
	<b>Frank Hovorka Assistant Professorship in Chemistry</b>	2012 – present
	Case Western Reserve University, Cleveland, OH	

#### **Honors and Awards**

- 1) Selected in the 40-40 Club (2010). Recognizes young Hispanic leaders in the Cleveland community.
- 2) Frank Hovorka Assistant Professor of Chemistry, Case Western Reserve University (2012).

#### **TEACHING / MENTORING**

##### **Courses Taught**

- CHEM 332: Laboratory Methods in Physical Chemistry, spring 2008, 2009, 2010, & 2011, 3 credit hours.
- CHEM 305: Introduction to Laboratory Methods in Physical Chemistry, spring 2009, 2010, & 2011, 3 credit hours.
- CHEM 446/337: Quantum Mechanics I, fall 2008 & 2010, 3 credit hours.
- CHEM 406: Chemical Kinetics, fall 2009 & 2011, 3 credit hours.
- CHEM 336: Physical Chemistry II, spring 2012

##### **Post Graduate Associates**

- 1) Dr. Amy Sage (02/01/2008 – 11/30/2008). Currently postdoctoral researcher at Kent State University, Department

of Chemistry, working with Prof. Shanhu Lee group.

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)

2) Chengwei Wen (start date 01/08/2008; Master's Plan B completed on 12/2011)

3) Cao Guo (start date 01/08/2009; Master's Plan B completed on 12/2011)

4) Qing Wang (start date 01/08/2009; Master's Plan B completed on 12/2011)

5) Huijuan Huang (start date 01/08/2010)

6) Nicholas Dunn (start date 01/08/2011)

7) Marvin Pollum (start date 01/08/2011)

#### **Undergraduate Students**

1) Jeff Lyvers (2008). Currently working in the Department of Pharmacology, Case Western School of Medicine.

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

3) Do-Yong Kim (2008 – 2009). Currently graduate student at Texas A&M University, Department of Chemistry, working with Prof. Simon W. North group.

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

5) Leah Dodson (2008 – 2010). Currently graduate student at California Institute of Technology, Department of Chemistry, working with Prof. Okomura group.

6) Saeed Rahman (2008 – 2010). Currently in Cambodia, Peace Corps.

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

8) Hannah Jenkins (2011 – present)

9) Veronica Laos (2011 – present)

#### **High School Students**

1) Courtney Johnson (summer 2008)

2) Matthew Beard (summer 2010; ACS-SEED Program)

3) Briana Sealey (summer 2011; ACS-SEED Program)

4) Omar Mahmoud (summer 2012; ACS-SEED Program)

5) Briana Sealey (summer 2012; ACS-SEED Program)

#### **Visiting Students**

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

2) Maria Morel (Ph.D. Student, University of Puerto Rico, San Juan Campus, 2009).

#### **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 – 2011). 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 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.

- Awardee and coordinator of the ACS SEED Summer Program (2010 & 2011). Summer research experience for economically disadvantage or underrepresented high school students in Cleveland.

## **SERVICE**

### ***Service to the University and Department***

- Ongoing collaboration with Ms. Churyl Croone, Assistant Director, International Student Recruitment Coordinator Territories: International Countries, to increase population of undergraduate students from Puerto Rico (2007– present).
- Ongoing collaboration with Mr. Joseph T. Williams, Director, Office of Multicultural Programs (2007– present).
- Member of the Chemistry Graduate Admissions Committee (2007– 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).
- Member of the Chemistry Visibility Committee (2011 – present).
- Reviewer for the CWRU Support of Undergraduate Research & Creative Endeavors (SOURCE) Program (2008 – present).
- Chair and organizer of the 2011 Graduate Chemistry Retreat (October 8, 2011). In this event, 4th-year graduate students present orally their research work to the faculty and to other graduate students in our department.
- PI and coordinator of the ACS SEED Summer Program. Summer research experience for economically disadvantage or underrepresented high school students in the greater Cleveland area (Summers 2010 & 2011).
- I collaborated with Ms. Lisa Dunnigan, Assistant Director and Coordinator of Multicultural Student Recruitment Programs, Office of Undergraduate Admission, CWRU (2008 – 2011). I participated on the Diversity Weekend Recruitment Brunch hosted by Undergraduate Admission.
- Member of the Chemistry Resources Committee (2008 – 2011).
- Member of the Energy and Material Science New Faculty Recruiting Committee (Spring 2008).
- Member of the Chemistry Executive Committee (2007 – 2008).

### ***Workshops Organized***

- 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.
- 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.
- Preparing and Delivering Scientific Talks (Fall 2011). As part of the 2011 Graduate Chemistry Retreat, I prepared 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***

- Editorial Board Member of the journal ISRN Spectroscopy (2011 – present).
- Committee Member of Grants and Awards for the American Society for Photobiology (2011 – present).
- Active reviewer of several scientific journals. These include: *Angewandte Chemie International Edition*, *Applied Physics Letters*, *Biochemistry*, *Chemical Communications*, *Chemical Physics Letters*, *ChemPhysChem*, *Journal of Chemical Physics*, *Journal of Computational and Theoretical Chemistry*, *Journal of Molecular Structure*, *Journal of Photochemistry and Photobiology*, *Journal of Physical Chemistry*, *Journal of the American Chemical Society*, *Langmuir*, *Physical Chemistry Chemical Physics*, *Photochemistry and Photobiology*, *Proceedings of the National Academy of Sciences*, and *Radiation*

Research.

- Active reviewer of proposals for the National Science Foundation including a 2009 NSF-MRI review panel, 2010 NSF-CRIF-MU review panel, 2012 NSF-CMI review panel, ACS Petroleum Research Fund, Research Corporation for Science Advancement (Cottrell College Science Award), and the Ohio Supercomputer Center.

#### **Conferences Organized**

- Symposium Chair: The 33<sup>rd</sup> American Society for Photobiology Meeting, Río Grande, Puerto Rico. Symposium title: 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.

### **RESEARCH / SCHOLARSHIP**

#### **Proposal and Award Activity**

*Omitted for web version.*

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

- Antonio E. Alegría, Department of Chemistry, University of Puerto Rico, Humacao, Puerto Rico, USA
- Rafael Arce, Department of Chemistry, University of Puerto Rico, San Juan, Puerto Rico, USA
- Gotard Burdzinski, Department of Physics, Adam Mickiewicz University, Poznan, Poland
- David Close, Department of Physics, East Tennessee State University, Johnson City, Tennessee, USA
- Carmelo García, Department of Chemistry, University of Puerto Rico, Humacao, Puerto Rico, USA
- 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
- Jerzy Leszczynski, Computational Center for Molecular Modeling Structure and Interactions, Department of Chemistry, Jackson State University, Jackson, Mississippi, USA
- Michael A. Meador, Polymeric Material Branch, NASA Glen Research Center, Cleveland, Ohio, USA
- Javier Santos-Pérez, Polymeric Material Branch, NASA Glen Research Center, Cleveland, Ohio, USA

#### **Publications** (\* = corresponding author)

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

1) 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.

2) O. Isayev; \* C. E. Crespo-Hernández; L. Gorb; F. C. Hil; J. Leszczynski; "In Silico Structure-Function Analysis of E. cloacae Nitroreductase", *Proteins* **2012**, DOI: 10.1002/prot.24157.

3) 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.

4) L. G. Dodson;† 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.

5) 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.

*Crespo, April 2012*

6) 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 Carboquinone", *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.

7) 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.

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

9) 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.

10) 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).

11) 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.

12) 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.

13) 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" (**Special Issue in Biophysics**), *ChemPhysChem* **2009**, 60, 1421-1425.

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) 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.

- 5) 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.
- 6) 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.
- 7) C. E. Crespo-Hernández; B. Cohen; B. Kohler,\* "Molecular spectroscopy: Complexity of Excited-State Dynamics in DNA (Replay)", *Nature* **2006**, 441, E7-E8.
- 8) 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.
- 9) 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.
- 10) C. E. Crespo-Hernández; B. Cohen; B. Kohler,\* "Base Stacking Controls Excited-State Dynamics in A-T-containing DNA", *Nature* **2005**, 436, 1141-1144.
- 11) 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.
- 12) 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.
- 13) 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.
- 14) 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.
- 15) C. Crespo-Hernández; R. Arce; E. Quiñones,\* "Magnetic Field Enhancement of the 6-Methylpurine Photoionization Yield", *Chem. Phys. Lett.* **2003**, 382, 661-664.
- 16) 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.
- 17) C. E. Crespo-Hernández; R. Arce,\* "Photoinization 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.
- 18) 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.
- 19) 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.

20) 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.

21) 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.

22) 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, Conference Proceedings, and Book Chapters**

1) R. A. Vogt; S. Rahman;† C. E. Crespo-Hernández,\* "Structure-Activity Relationships in Nitro-Aromatic Compounds" (*Invited*), 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.

2) 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.

3) 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.

4) 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.

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

### **Invited Oral Presentations (May, 2006 – present)**

1) Excited-State Dynamics in Nucleic Acids Analogues, Astrobiology Science Conference 2012, Atlanta, Georgia, April 16-20, 2012.

2) Does DNA Dynamics Come in Singlet and Triplet Flavors?, Jackson State University, Department of Chemistry, Jackson, Mississippi, October 8, 2010.

3) Time-Resolved Photochemistry of DNA, University of Akron, Department of Chemistry, September 14, 2010.

4) Shining Light on the Molecule of Life, 35<sup>th</sup> American Society for Photobiology Meeting, Providence, Rhode Island, June 12-16, 2010.

5) Shining Light on the Molecule of Life, Calvin College, Department of Chemistry, Grand Rapids, Michigan, March 4, 2010.

6) Shining Light on the Molecule of Life, Hope College, Department of Chemistry, Holland, Michigan, March 5, 2010.

- 7) Time-Resolved Photochemistry of DNA, Case Western Reserve University, NIH/NHLBIT35 Program, School of Medicine, Cleveland, Ohio, June 10, 2009.
- 8) Ultrafast Dynamics of Biomolecules and Nitro-Aromatic Compounds, Jackson State University, Department of Chemistry, Jackson, Mississippi, March 27, 2009.
- 9) DNA Photodynamics: From Single Bases to the Double Helix, Case Western Reserve University, School of Medicine, Department of Biochemistry, Cleveland, Ohio, October 30, 2008.
- 10) Probing DNA Electronic Energy Flow and Its Mutagenic Consequences, Department of Chemistry, Cleveland State University, Cleveland, Ohio, October 10, 2008.
- 11) Academy as a Professional Career Path for Underrepresented Groups in Sciences, Case Western Reserve University, T35 Minority Training Grant, School of Medicine, Cleveland, Ohio, June 11, 2008.
- 12) 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.
- 13) Academy as a Professional Career Path, Case Western Reserve University, School of Medicine, Minority Graduate Student Organization, Cleveland, Ohio, January 18, 2008.
- 14) 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.
- 15) 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 16-20, 2007.
- 16) Relaxation of Excess Electronic Energy and Ultrafast Formation of Thymine-Thymine Photodimer in DNA, Case Western Reserve University, Cleveland, Ohio, January 30, 2007.
- 17) Excited State Dynamics in Nucleic Acid Monomers and Polymers: UV-Induced Ultrafast Formation of Thymine-Thymine Photodimer in DNA, University of Houston, Houston, Texas, January 11, 2007.
- 18) Ultrafast Excited State Dynamics: Direct Observation of DNA Damage by UV Light; University of Miami, Coral Gables, Miami, January 4, 2007.
- 19) Ultrafast Energy Relaxation in Biomolecules: Real Time Observation of DNA Damage by UV Light; University of North Carolina, Chapel Hills, North Carolina, December 18, 2006.
- 20) From Femtochemistry to Femtobiology: Direct Observation of Excited State Dynamics and DNA Damage by UV Light; University of Kansas, Kansas City, Kansas, December 14, 2006.
- 21) Early Events in DNA Photophysics; 17<sup>th</sup> Inter-American Photochemical Society Conference on Photochemistry, Salvador, Bahia, Brazil, June 11-June 16, 2006.
- 22) Real Time Observation of DNA Damage by Ultraviolet Radiation: New Insights Half a Century After Watson-Crick's Discovery of Double Stranded DNA; University of Puerto Rico, San Juan Campus, San Juan, Puerto Rico, May 16, 2006.



**Contributed Oral Presentations** (May, 2003 – present)

- 1) UVA-Induced Dynamics in Sulfur-Substituted Nucleosides, 36<sup>th</sup> American Society for Photobiology Meeting, Montreal, Canada, June 23 to 27, 2012.
- 2) Solvent Relaxation Following Vibrational Cooling in the Triplet Manifold of 1-Nitronaphthalene, XXIV International Conference on Photochemistry, Toledo, Spain, July 19 to 24, 2009.
- 3) 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 – September 1, 2005.
- 4) 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 20-24, 2005.
- 5) 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 20-22, 2005.
- 6) Research in Kohler's Group, Autumn Research Presentation to First Year Graduate Students, Department of Chemistry, The Ohio State University, October 14, 2004.
- 7) *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 26-27, 2004.
- 8) 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 5-9, 2003.
- 9) Photophysics of DNA and RNA Polymers Studied by Femtosecond Pump-Probe Spectroscopy, The 2<sup>nd</sup> Ohio Photochemical Society Meeting, Ohio, USA, May 16-18, 2003.

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- 1) M. Pollum; C. E. Crespo-Hernández, "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.
- 2) C. E. Crespo-Hernández; Huang, H.; Vogt, R. A.; Isayev, O., "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.
- 3) R. A. Vogt; C. Reichardt; C. E. Crespo-Hernández, T. G. Gray, "Ultrafast Dynamics in Nitro- and (Organophosphine)Gold(I)-Polycyclic Aromatic Hydrocarbons", 2011 Meeting in Miniature, Ursuline College, Pepper Pike, Ohio, March 16, 2011.
- 4) C. Wen; C. Reichardt; C. E. Crespo-Hernández, "Excited-State Dynamics in 2-Aminopurine Ribonucleoside: From Femtosecond to Microsecond Time Scale", 66<sup>th</sup> International Symposium on Molecular Spectroscopy, The Ohio State University, Columbus, Ohio, June 20-24, 2011.
- 5) R. A. Vogt; C. Reichardt; C. E. Crespo-Hernández, T. G. Gray, "Ultrafast Dynamics in Nitro- and (Organophosphine)Gold(I)-Polycyclic Aromatic Hydrocarbons", 66<sup>th</sup> International Symposium on Molecular Spectroscopy, The Ohio State University, Columbus, Ohio, June 20-24, 2011.
- 6) 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.

7) 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.

8) 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.

9) 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.

10) 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.

11) 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.

12) 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.

13) 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.

14) 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.

(\* **First Place Winner in Natural Sciences Poster Competition**). † participated as undergraduate student.

15) 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.

16) 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.

17) 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.

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

18) 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.

19) 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.

- 20) 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.
- 21) 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.
- 22) 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.
- 23) 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.
- 24) 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.
- 25) 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.
- 26) 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.
- 27) 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.
- 28) B. Kohler; T. Takaya; C. Su; C. E. Crespo-Hernández, “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.
- 29) K. D. de La Harpe; C. E. Crespo-Hernández; 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.