Carlos E. Crespo-Hernández **Curriculum Vitae**

Case Western Reserve University
Department of Chemistry **Phone: (216)-368-1911**
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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

Assistant Professor of Chemistry *2007*
Case Western Reserve University, Cleveland, OH

Current Graduate Students

1) Robert Aaron Vogt (start date 11/2007)

Post-Graduate Associates

1) Dr. Amy Sage (02/2008)
2) Dr. Chirstian Reichardt (03/2008)

Current Undergraduate Students

1) Leah Dodson
2) Bradley Sutton
3) Jeffrey Lyvers
4) Do-Yong Kim

Recent Synergistic Activities

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

- The PI is an active participant in the training of groups underrepresented in science.
- Associated Faculty of the Minority Graduate Student Organization (MGSO) at Case Western Reserve University (2007). 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.
- Underrepresented 8th and 9th graders, 2007-2008. In fall 2008, the PI will be participating in a series of 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 is to strength STEM concepts and motivates students to follow STEM career path in the future. This is a joint effort with Dr. LaShanda Korley, African-American and Assistant Professor of Macromolecular Science and Engineering Department at Case Western Reserve University.

- Puerto Rico Graduate Teaching Fellows in K-12 Education sponsored by the National Science Foundation at the University of Puerto Rico, San Juan Campus, Puerto Rico, 2000-2002. The PI developed and offered lectures to strengthen and reinforced STEM concepts to K-12 students in public schools using constructivism, cooperative work, and discovery as theories for teaching and learning. The PI also strengthens STEM concepts and modeled effective teaching theories to K-12 teachers in public school in Puerto Rico.
- Minority Graduate Education Program sponsored by the National Science Foundation at the University of Puerto Rico, San Juan Campus, Puerto Rico, 1999-2001. The PI mentored and supported several first year graduate students in chemistry.

Service to the Scientific and Engineering Community Outside of the PI's Immediate Organization

- The PI is an active reviewer of several scientific journals. These include: Applied Physics, Biochemistry, Journal of Molecular Structure, Journal of Photochemistry and Photobiology, Journal of Physical Chemistry, Journal of the American Chemical Society, Langmuir, Photochemistry and Photobiology, and Radiation Research.
- The PI is an active reviewer of proposals for the National Science Foundation and Ohio Supercomputer Center.

Service to the PI's 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.
- Member of the Chemistry Executive Committee.
- Member of the Chemistry Graduate Recruiting Committee.
- Member of the Energy and Material Science New faculty Recruiting Committee.

Conferences organized

- Symposium Chair: The 33rd 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.

Collaborators

- Bern Kohler, Department of Chemistry, The Ohio State University, Columbus, Ohio, USA
- Carmelo García, Department of Chemistry, University of Puerto Rico, Humacao, 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
- Jerzy Leszczynski, Department of Chemistry, Jackson State University, Jackson, Mississippi, USA
- Leonid Gorb, Department of Molecular Biophysics, Institute of Molecular Biology and Genetics, National Academy of Science of Ukraine, Kyiv, Ukraine
- Rafael Arce, Department of Chemistry, University of Puerto Rico, San Juan, Puerto Rico, USA

Courses Taught

- CHEM 332: Laboratory Methods in Physical Chemistry, spring 2008, 3 credit hours.

Current and Pending Funding Activities

- **Omitted for the web version.**

Professional Societies and Memberships

- Optical Society of America
- American Society for Photobiology
- American Chemical Society

Publications

1) L. Yu Kay; J. Azadi; C. E. Crespo-Hernández; E. Olmon; B. Kohler; "Prediction of Thymine Dimerization Yields from Molecular Dynamics Simulations", *Biophysical J.* **2008**, *in press.*

2) Close, D. M.; 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**, *in press.*

3) C. E. Crespo-Hernández;* C. N. J. Marai, "Vertical Singlet Excitations on Adenine Dimer: A Time Dependent Density Functional Study", *American Institute of Physics Conference Proceedings (AIP Conference Proceedings)*, **2007**, 963, 607-610. *Corresponding author.

4) 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. *Corresponding author.

5) 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.

6) 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.

7) P. M. Hare; C. E. Crespo-Hernández; B. Kohler, "Solvent-Dependent Photophysics of 1-cyclohexyluracil: Ultrafast Branching in the Initial Bright State Leads Nonradiatively to the Electronic Ground State and a Long-Lived $^1n\pi$ State", *J. Phys. Chem. B* **2006**, 110, 18641-18650.

8) L. Colón; C. E. Crespo-Hernández;* R. Oyola; C. García; R. Arce,* "Photochemical and Photophysical Properties of the A·T Sequence Isomers: An Experimental and Theoretical Approach", *J. Phys. Chem. B* **2006**, 110, 15589-15596. *Corresponding authors.

9) C. E. Crespo-Hernández; B. Cohen; B. Kohler, "Molecular spectroscopy: Complexity of Excited-State Dynamics in DNA (Replay)", *Nature (Brief Communications Arising)* **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. *Corresponding authors.

16) 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.

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

18) 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.

19) C. Crespo-Hernández; R. Arce; E. Quiñones, "Magnetic Field Enhancement of the 6-Methylpurine Photoionization Yield", *Chem. Phys. Lett.* **2003**, 382, 661-664.

20) 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.

21) 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.

22) 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.

23) C. E. Crespo-Hernández, "Photochemical studies of DNA and RNA Bases, Nucleosides, Nucleotides, and Dinucleotides", Dissertation, University of Puerto Rico, Río Piedras, Puerto Rico, UMI, Order No. DA3083759, **2002**, CAN 141:309127, AN 2004:104500.

24) 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.

25) 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.

26) 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.

27) 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.

Invited Talk Presentations

1) Academy as a Professional Career Path, Case Western Reserve University, School of Medicine, Minority Graduate Student Organization, Cleveland, Ohio, January 11, 2008.

2) 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.

3) 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.

4) Relaxation of Excess Electronic Energy and Ultrafast Formation of Thymine-Thymine Photodimer in DNA, Case Western Reserve University, Cleveland, Ohio, January 30, 2007.

5) 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.

6) Ultrafast Excited State Dynamics: Direct Observation of DNA Damage by UV Light; University of Miami, Coral Gables, Miami, January 4, 2007.

7) 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.

8) 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.

9) Early Events in DNA Photophysics; 17th Inter-American Photochemical Society Conference on Photochemistry, Salvador, Bahía, Brazil, June 11-June 16, 2006.

10) 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.

Selected Oral Presentations (20 in total)

1) Early Events in DNA Photophysics; presented by C. E. Crespo-Hernández and Bern Kohler at the 17th Inter-American Photochemical Society Conference on Photochemistry, Salvador, Bahía, Brazil, June 11-June 16, 2006.

2) Real Time Observation of DNA Damage by Ultraviolet Radiation: New Insights Half a Century After Watson-Crick's Discovery of Double Stranded DNA; presented by C. E. Crespo-Hernández, University of Puerto Rico, Río Piedras Campus, San Juan, Puerto Rico, May 16, 2006.

3) Base stacking, not base pairing, governs excited-state dynamics in A·T-containing DNA; presented by C. E. Crespo-Hernández and Bern Kohler at The 230th 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; presented by C. E. Crespo-Hernández and Bern Kohler at 60th 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; presented by C. E. Crespo-Hernández and Bern Kohler at 4th Meeting of the Ohio Photochemical Society, Oxford, Ohio, May 20-22, 2005.

6) Research in Kohler's Group; presented by C. E. Crespo-Hernández, 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; presented by C. E. Crespo-Hernández, Rafael Arce, Yasuyuki Ishikawa, Leonid Gorb, Jerzy Leszczynski, and David M. Close at the 4th 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; presented by C. E. Crespo-Hernández and Bern Kohler at The 31st 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; presented by C. E. Crespo-Hernández and Bern Kohler at The 2nd Ohio Photochemical Society Meeting, Ohio, USA, May 16-18, 2003.

10) Determination of Trace Concentrations of Actinides in the NIST Bone Ash Standard Reference Material Using TRU-Spec Extraction Resin, presented by C. Crespo, Zhichao Lin and Kenneth G. W. Inn at 45th Annual Conference on Bioassay, Analytical, and Environmental Radiochemistry, Boston, November 13-16, 1995.