Claudio Carra, Ph.D.

Resume

SUMMARY

Talented and accomplished **Research Scientist**, coauthor of more than twenty peer reviewed papers, with extensive background in biochemistry, biology, physical, organic, and theoretical chemistry. International experiences in Canada, US, and Europe. Ph.D. in Physical Chemistry. Post-doctoral research in computational chemistry, with emphasis on modeling chemical systems of technological and biological interest. Current experience in instructing undergraduate classes and laboratories.

EDUCATION

University of Fribourg, Fribourg, Switzerland; ***Ph.D. in Physical Chemistry*** *(2001)*
Thesis: "Spectroscopic and Theoretical Study of Reactive Intermediates Generated in Cryogenic Matrices by Photolysis and Radiolysis"
University of Torino, Torino, Italy; ***M.S. in Organic Chemistry****, graduated cum laude (1995)*
Thesis: "*Ab initio* theoretical study of mesolytic cleavage of radical anions and radical cations"

PROFESSIONAL & RESEARCH EXPERIENCE

University of Houston Downtown, Chemistry Faculty, Houston, TX 2012 – Present
Adjunct Faculty Member

- Teaching courses of General Chemistry laboratories.

Houston Community College, Chemistry Faculty, Houston, TX 2009 – Present
Adjunct Faculty Member

- Teaching courses of General Chemistry II, introduction to chemistry and biology. 2006 – 2012

Research Scientists

- The research focuses on the modeling of the activity of the recombinases enzymes, main promoters for the repair of DNA damages due to space radiation. The systems investigated are the RecA for prokaryotes, RPA for eukaryotes and humans. The study is performed by using theoretical and experimental tools.

University of Ottawa, Ottawa, ON 2003 – 2006
Postdoctoral Research Assistant

- Investigated origin of interaction of fluorescent dyes with single and double-strand DNA, using molecular classical dynamics, to understand behaviors which might lead to design of more efficient fluorescent probes to detect DNA chain damages.
- Performed a theoretical study on ground and excited states, using multi configurational quantum chemical methods, on reactions carried out by laser flash photolysis.
- Modeled by Density Functional Theory (DFT), alkyl and aryl boron center radical reactions, interaction between zeolite frameworks and guest molecule, solvated organic ions, and photocages.
- Instructed undergraduate classes in Introduction to Quantum Chemistry.

Penn State University, State College, PA 2001 – 2003
Postdoctoral Research Assistant

- Conducted theoretical studies on proton-coupled electron transfer (PCET) in biological systems.
- Demonstrated that mechanism of hydrogen transfer can be PCET or single electron transfer (ET) in function of value of pH.
- Performed theoretical calculations on model system for tyrosine oxidation in photosystem II.
- Modeled PCET process in radical anionic thymine-acrylamide complex in DNA system.

University of Fribourg, Fribourg, Switzerland 1997 – 2001
Ph.D. Candidate

- Carried out extensive studies under Professor T. Bally focused on characterizing new reactive intermediates observed in reactions in a solid inert medium kept at low temperature to prevent diffusion and thermal decomposition. The reactive intermediates are generated by photolysis to produce neutral fragmentations, or generated by X-irradiation to produce corresponding radical cations.
- Reproduced experimental spectra and performed theoretical modeling of the observed chemical processes, utilizing various methods implemented in quantum chemical programs.
- Instructed undergraduate classes and laboratories in Physical Chemistry.
- Thesis advisor for four graduate students in Physical Chemistry.

Ecole Polytechnique, Paris, France 1994 – 1995
Student Research Program

- Selected to participate in research at Département de Chimie Laboratoire des Mécanismes Réactionnels on study grant from ERASMUS Program (European Community Action Scheme for the Mobility of University Students). Study involved quantitative estimation of binding energies of organic substrates on metal centers to describe process mechanisms and characterize the geometries of the species involved.

PROFESSIONAL DEVELOPMENT

- Quantum Chemistry, European Summerschool in Quantum Chemistry, Riolo Terme, Italy (2000)
- Modern Methods and Algorithms of Quantum Chemistry, Jülich, Germany (2000)
- European School of Computational Chemistry Reaction and Molecular Dynamics, Università degli Studi di Perugia, Perugia, Italy (1999)
- Introduction to Gaussian: Theory and Practice Roma, Italy (1998)
- Teaching Large Classes, Learning to Teach from Within, Disruptive Student Behavior, University of Ottawa, Ontario (2003-2005)

INVITED LECTURES

- "DNA Recombinase Protein of the *E. coli*, its Function and Structure in the Active Form, a Computational Study", South Western State University, Americus, GA, September 4-5, 2008.
- Theory and Applications of Computational Chemistry (TACC), Shanghai, China, September 23-27, 2008 (declined).
- "DNA Recombinase Proteins, their Function and Structure in the Active Form, a Computational Study", Molecular Modeling Group at the Indian Institute of Chemical Technology, Hyderabad, India, June 1-11, 2007

TECHNICAL SKILLS

Laboratories: Extensive experience in using FR-IR, UV-Vis, GC-MS, NMR, and the most standard chemical equipments.
Linux: Administrator level. Modeling packages: Gaussian, Molcas, Access II, Molpro, Dalton, Gamess, Amber, GaussView, GopenMol, Molekel, Moplot, Molden, VMD, PyMol.
Windows: Administrator level. MS Office package, ChemDraw, Pow-Ray, Corel Draw, MatLab.
Languages: Fluent in Italian, English, and French.

CITIZENSHIP

Italian, US Permanent Resident

PUBLICATIONS

1. C. Carra, J. Saha, F. A. Cucinotta, "Theoretical Prediction of the Binding Free Energy for Mutants of Replication Protein A", *J. Mol. Model.*, **2012**, *12*, 3035-3049

2. C. Carra, F. A. Cucinotta, "Accurate Prediction of the Binding Free Energy and Analysis of the Mechanism of the Interaction of Replication Protein A (RPA) with ssDNA", *J. Mol. Model*., **2011**, 17, 133-150,
3. S. Rajam, R. S. Murthy, A. V. Jadhav, Q. Li, C. Keller, C. Carra, T. C. S. Pace, C. Bohne, B. S. Ault, A. D. Gudmundsdottir, "Photolysis of (3-Methyl-2H-azirin-2-yl)-Phenylmethanone: Direct Detection of a Triplet Vinylnitrene Intermediate", *J. Org. Chem.*, **2011,** *76*(24), 9934
4. C. Carra, F. A. Cucinotta, "Binding sites of the E. Coli DNA recombinase protein to the ssDNA: a computational study", *J Biomol. Struct. Dyn.*, **2010**; *27*, 407-28
5. C. Carra, F. A. Cucinotta, "Selectivity of DNA Recombinase Protein, a Computational Approach", *J. Mol. Model.,* **2010**; (17), 133-150.
6. C. Carra, J. C. Scaiano" Nucleohomolytic Substitution at Boron: A Computational Approach", *Eur. J. Org. Chem*., **2008**, *(26)*, 4454 - 4459
7. J.C. Conrad, M. Kotyk, C. Carra, S.I. Gorelsky*, D.E. Fogg*, " Geometric and Electronic Structure of a C_1-Symmetric Ru-Aryloxide Metathesis Catalyst: An Experimental and Computational Study", *Organometallics* **2009**, *28*, 5424–5431.
8. P. Antoniotti, C. Carra, A. Maranzana, G. Tonachini, "Germyl mesolytic dissociations in the allylgermane and penta- 2,4-dienylgermane radical anions. A theoretical study", *Theor Chem Account*, **2007**, (118), 253-264
9. J. Wang, G. Burdzinski, Z. Zhu, M. S. Platz, C. Carra, T. Bally "Ultrafast Spectroscopic and Matrix Isolation Studies of *p*-Biphenylyl, *o*-Biphenylyl, and 1-Naphthylnitrenium Cations", *J. Am. Chem. Soc*., **2007**; *129(26)*, 8380-8388.
10. M. Perry, C. Carra, M. Chretien, J. C. Scaiano, "Effect of Hexafluorobenzene on the Photophysics of Pyrene", *J. Phys. Chem. A*., **2007**, *111(23)*, 4884-4889.
11. C. Carra, R. Nussbaum, T. Bally "Experimental and Theoretical Study of 2,6-Difluorophenylnitrene, Its Radical Cation, and Their Rearrangement Products in Argon Matrices", *Chem. Phys. Chem.*, **2006**, *7*, 1268 – 1275.
12. L. Mikelsons, C. Carra, M. Shaw, C. Schweitzer, J. C. Scaiano "Experimental and Theoretical Study of the Interaction of Single-Stranded DNA Homopolymers and a Monomethine Cyanine Dye: Nature of Specific Binding", *Photochem. Photobiol. Sci.*, **2005**, *4(10)*, 798-802.
13. C. Carra, T. Bally, A. Albini "Role of Conformation and Electronic Structure in the Chemistry of Ground and Excited State o-Pyrazolylphenylnitrenes", *J. Am. Chem. Soc*. **2005**, *127*, 5552 -5562.
14. C. Carra, N. Iordanova, S. Hammes-Schiffer, ""Proton-Coupled Electron Transfer in a model for Thyrosine Oxidation in Photosystem II", *J. Am. Chem. Soc.*, **2003**, *125*, 10429-10436.
15. C. Carra, G. Ghigo, G. Tonachini, "Methyl and Silyl Mesolytic Dissociations in Radical Cations and Radical Anions of But-1-ene, Allylsilane, Hexa-1,3-diene, and Penta-2,4-dienylsilane. CAS-MCSCF and Coupled Cluster Theoretical Study", *J. Org. Chem*, **2003**, *68*, 6083-6095.
16. C. Carra, N. Iordanova, S. Hammes-Schiffer, "Proton-Coupled Electron Transfer in DNA-Acrylamide Complexes", *J. Phys. Chem. B*, **2002**, 8415-8421.
17. C. Carra, T. Bally, T. A. Jenny and A. Albini, "Thermoreversible Photocyclization of a Pyrazolotriazole to a Triazasemibullvalene: a Novel Electrocyclic Eeaction", *Photochem. Photobiol. Sci.*, **2002**, *1*, 1-7.
18. K. Schroeter, D. Schröder, H. Schwarz, G. D. Reddy, O. Wiest, C. Carra, and T. Bally, "Ion Chemistry of anti-*o,o'*-Dibenzene", *Chem. Eur. J.*, **2000**, *6*, 4422-4430.
19. T. Bally, C. Carra, S. Matzinger, L. Truttmann, F. Gerson, R. Schmidlin, M. S. Platz, and A. Admasu,"π- and σ-Diazo Radical Cations: Electronic and Molecular Structure of a Chemical Chameleon", *J. Am. Chem. Soc*., **1999**, *121*, 7011-7019.
20. T. Bally, C. Carra, M. P. Fülscher and Z. Zhu, "Electronic Structure of the Naphthalene Radical Cation and Some Simple Alkylated Derivatives", *J. Chem. Soc., Perking Trans. 2*, **1998**, 1759-1765.
21. C. Carra, F. Fiussello, and G. Tonachini, "Nature of Methyl and Silyl Mesolytic Dissociations in Substituted Cyclopropenyl Radical Cations and Anions. A CAS-MCSCF and CCSD(T) Theoretical Study", *J. Org. Chem.*, **1999**, *64*, 3867-3877.

22. F. Bouchard, V. Brenner, C. Carra, J. W. Hepburn, G. K. Koyanagi, T. B. McMahon, G. Ohanessian, and M. Peschke, "Energetics and Structure of Complexes of Al^+ with Small Organic Molecules in the Gas Phase", *J. Phys. Chem. A*, **1997**, *101*, 5885-5894.

PRESENTATIONS, POSTERS, & CONTRIBUTIONS

- September 18–21, 2011, The 22nd Annual NASA Space Radiation Investigators' Workshop, League City, TX; C. Carra*, F. A. Cucinotta: "Accurate Prediction of the Binding Free Energy and Analysis of the Mechanism of the Interaction of Replication Protein A (RPA) with ssDNA".
- May 15-19, 2010, 11th International Workshop on Radiation Damage to DNA, Atlanta, Georgia; C. Carra*, F. A. Cucinotta: "Selectivity and Binding Mechanism of *E. coli* DNA recombinase Protein, a Computational Approach".
- March 21-26, 2010, Gordon Conference: DNA Damage, Mutation & Cancer, Ventura, CA; C. Carra*, F. A. Cucinotta: "Selectivity and Binding of *E. coli* Recombinase Protein, a Rheoretical Approach"
- September 14-19, 2008, WATOC 2008, Sydney Australia; C. Carra*, F. A. Cucinotta, "The binding modes of DNA Recombinase Protein of the *E. coli*, a Computational Study".
- May 18-19, 2008, Galveston Texas, Structural Biology Symposium; C. Carra*, F. A. Cucinotta, "DNA Recombinase Protein of the *Mycobacterium Tuberculosis*, its Function and Structure in the Active Form, a Computational Study".
- July 8-13, 2007, Gordon Conference: ENZYMES, COENZYMES & METABOLIC PATHWAYS, University of New England, Biddeford, ME; C. Carra*, F. A. Cucinotta, "DNA Recombinase Proteins, their Function and Structure in the Active Form, a Computational Study".
- January 16-21, 2005: WATOC 2005. Modelling Structure and Reactivity, Cape Town, South Africa; talk: C.Carra*, L. Mikelsons, M. Shaw, J.C. Scaiano, "Nanosecond Molecular Dynamics Simulations and Structural Analysis of dsDNA-dye Complex in Solution".
- July 13-18, 2002: American Conference on Theoretical Chemistry, Champion, PA; C. Carra*, N. Iordanova, S. Hammes-Schiffer, "Theoretical Studies of Proton-Coupled Electron Transfer Reactions".
- August 26-31, 2000: Conference on Reactive Intermediates and Unusual Molecules Vienna, Austria; C. Carra*, T. Bally, A. Albini, "Photochemical Intramolecular Trapping of Azidophenyl Pyrazoles at Low Temperature Ar Matrices".
- February 21-25, 2000: Winterschool: Modern Methods and Algorithms of Quantum Chemistry, Jülich, Germany; C. Carra*, T. Bally, O. G. Wiest, "Reactivity of anti-o,o'-Dibenzene Radical Cation in Argon Matrix".
- September 6-10, 1999: 8th International Conference on the Applications of DFT to Chemistry and Physics DFT99 Roma, Italy.
- August 22-27, 1999: International Workshop on Reactive Intermediates, IWRI'99 Szczyrk, Poland; C. Carra*, T. Bally, M. S. Platz, Z. Zhu, "Electronic and Vibrational Spectra of Some Arylnitrenium Ions in Low temperature Matrices".
- May 30-June 3, 1999: Giornate di Chimica Organica Fisica e Meccanicistica, COFEM99, Mattinata (Foggia), Italy; C. Carra*, R. Giachino, G. Tonachini, "Processi di Scissione Mesolitica in Radicali Ioni Organici Insaturi. Studio Teorico".
- July 12-17, 1998: International Conference on Reactive Intermediates and Reaction Mechanisms Centro Stefano Franscini, Ascona, Switzerland; C. Carra*, Z. Zhu, T. Bally, M. P. Fülscher, "Electronic Structure of the Naphtalene Radical Cation and Some Simple Alkylated Derivatives".