

University of South Florida
Department of Chemistry
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Alfredo Cardenas, Ph.D.

Education

Postdoctoral Fellow *Cornell University, Ithaca, NY 2003*
Research Advisor: Prof. Ron Elber, Dept. of Computer Science

Ph.D., Chemistry *University of Pittsburgh, Pittsburgh, PA 2000*
Doctoral Advisor: Prof. Rob Coalson, Dept. of Chemistry
Dissertation Title: *Theoretical studies in multidimensional quantum systems and ionic permeation through biological channels*

M.S., Chemistry *Simon Bolivar University, Caracas, Venezuela 1993*

B.S., Chemistry (cum laude) *Simon Bolivar University, Caracas, Venezuela 1988*

Professional Experience

2003– Present *University of South Florida* *Assistant Professor*

1993-1994 *Simon Bolivar University* *Instructor Professor*

Research Interests

We use approximate algorithms based on a boundary value formulation of classical mechanics to study long time dynamical events like folding process of proteins, gating mechanisms of ion channels, conformational changes associated with signal transduction and function and ligand binding.

Research in progress

1. Clarke A, Urahata SM and Cardenas AE: More than 60 folding trajectories for three members of the cold shock protein family has been obtained and most of the analysis has been concluded.
2. Dametto, M and Cardenas AE: Several trajectories describing the folding process of apomyoglobin were obtained starting with an unfolded conformation from high temperature simulations. Similar computations under low pH conditions will be performed for comparison.
3. Hamm S and Cardenas AE: Influence of mutations in the folded process of Amyotropic Lateral

Sclerosis-related Cu,Zn-superoxide dismutase protein. Preliminary results have been obtained describing folding of monomeric, dimeric and reduced forms of the protein.

4. Aristide K, Rodriguez J, Hamm S, Larsen, R and Cardenas, AE: We have performed molecular simulations connecting ligand-bound and unbound forms of three oxygen sensing enzymes (FixL, Hem At and EcDos). This project has involved undergraduate students from the REU program.

5. Yu Y.X, and Cardenas, A.E. Use of robotic-motion planning techniques (graph methods) to improve the sampling of approximate boundary-value trajectories by optimization of the action.

Publications

A. RESEARCH ARTICLES

1. Cardenas, A.E., Elber, R, Atomically detailed simulations of helix formation with the stochastic difference equation. *Biophys. J.* 2003, *85*, 2919.
2. Cardenas, A.E., Elber, R, Kinetics of cytochrome c folding: Atomically detailed simulations. *Proteins* 2003, *51*, 245.
3. Elber, R, Cardenas, A, Ghosh, A. Stern, H.A, Bridging the gap between long time trajectories and reaction pathways. *Adv. Chem. Phys.* 2003, *126*, 93.
4. Elber, R.; Ghosh, A.; Cardenas, A. Long time dynamics of complex systems. *Acc. Chem. Res.* 2002, *35*, 396.
5. Chern, S.-S.; Cardenas, A.E.; Coalson, R.D. Three-dimensional dynamic Monte Carlo simulations of driven polymer transport through a hole in a wall. *J. Chem. Phys.* 2001, *115*, 7772.
6. Cardenas, A.E.; Coalson R.D.; Kurnikova, M. 3D Poisson-Nernst-Planck Theory Studies: Influence of Membrane Electrostatics on Gramicidin A Channel Conductance. *Biophys. J.* 2000, *79*, 80.
7. Cardenas, A.E.; Krems, R.; Coalson, R.D. Semiclassical Wave Packet Dynamics with Electronic Structure Computed on the Fly: Application to Photophysics of Electronic Excited States in Condensed Phase. *J. Phys. Chem. A* 1999 *103*, 9469.
8. Cardenas, A.E.; Coalson, R.D. Calculation of Reduced Partial Cross Sections of Molecules Photodesorbing from a Crystal Surface with Internal Vibrations: Inclusion of Curve-Crossing Effects. *J. Chem. Phys.* 1999, *110*, 11542.
9. Cardenas, A.E.; Coalson, R.D. A wavepacket-path integral method for curve-crossing problems: Application to resonance Raman spectra and photodissociation cross sections. *Chem. Phys. Lett.* 1997, *265*, 71.
10. Bessega, M.C.; Paz, J.L.; Hernández, A.J.; Cardenas, A.E. Study of additional resonances in frequency space and permanent dipole moment effects on nondegenerate four wave mixing signals. *Phys. Lett. A* 1995, *206*, 305.
11. Paz, J.L.; Bessega, M.C.; Cardenas, A.E.; Hernández, A.J. Study and characterization of new resonances in the frequency space in a two level system with non zero permanent dipole moments. *J. Phys. B* 1995, *28*, 5377.

12. Von Bergen, R.; Von Bergen, Y.; Rogel, E.; Cuetos, L.; Cardenas, A. Some considerations on Sanchez-Lacombe equation of state parameters. *Anales de Química (Spain)* 1995, *91 Supplements*, 623.
13. Paz, J.L.; Cardenas, A.E.; Hernández, A.J. Study and characterization of the four-wave mixing signal in the frequency space. *J. Phys. B* 1994, *28*, 5097.
14. Cardenas, A.E.; Paz, J.L.; Hernández, A.J. Study of the absorptive and dispersive responses on the resonant non-degenerate four-wave mixing signal. *Revista Mexicana de Física* 1994, *40*, 242.
15. Paz, J.L.; Cardenas, A.E.; Hernández, A.J.; Franco, H.J. Effects of the spectral inhomogeneity on the approximation levels for the study of the propagation of the Rayleigh type optical mixing signal. *Optics Communications* 1994, *109*, 195.
16. Paz, J.L.; Cardenas, A.E.; Hernández, A.J. Effects of solute concentration, field intensity and spectral inhomogeneous broadening on four-wave mixing. *Quantum Optics* 1993, *5*, 355.

B. BOOK CHAPTERS

1. Cardenas, A.E. and Barth E., Extending the timescale in atomically detailed simulations in *Reviews in Computational Chemistry*, K.B. Lipkowitz and D.B. Boyd, Editors, Wiley, New York (submitted).
2. Clarke, A.S, Hamm S.M. and Cardenas A.E., Extending atomistic time scale simulations by optimization of the action, in *Annual Reports in Computational Chemistry*, D. C. Spellmeyer Editor; Elsevier, Amsterdam (in press).
3. Elber, R.; Ghosh, A.; Cardenas, A, The Stochastic Difference Equation as a tool to compute long time dynamics a chapter *in Bridging the time scale gap*, Editors: Peter Nielaba, Michel Mareschal and Giovanni Ciccotti, Springer Verlag, Berlin, 2002.

Honors and Awards

2006	University of South Florida	Outstanding Research Achievement Award
2005	University of South Florida	Research Rising Stars

1998-2000	University of Pittsburgh	Andrew Mellon Predoctoral Fellowship
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1986-1994 Simon Bolivar University:

- Honorable Mention for the Annual Prize to the Best Scientific Research in Chemistry, National Council of Scientific and Technological Research of Venezuela
- Master Thesis with Distinguished Diploma, Simón Bolívar University
- Partial funding for the realization of Master Thesis, National Council of Scientific and Technological Research of Venezuela
- B.S., Scholarship, Cepet Petroleum Company of Venezuela.
- B.S., Scholarship, Corpoven Petroleum Company of Venezuela

Research Support

1. Agency: NSF
Amount: \$615,415
Duration: May 1, 2005 – April 30, 2010
Title: *CAREER: Biomolecular Simulations Coming to Age: Folding of Globular and Membrane-bound Proteins Studied by Computer.*
2. Agency: Research Council, New Researcher Grant, University of South Florida
Amount: \$8,650
Duration: January 1, 2004-December 31, 2004
Title: *Fast transition events and folding of small proteins studied with the stochastic difference equation in length algorithm*
3. Agency: Faculty Development Committee, University of South Florida
Amount: \$500
Duration: May 1, 2004-December 31, 2004
Title: *Folding simulations of apomyoglobin. Structural determinants of the folding process*

Presentations

A. POSTERS PRESENTED AT CONFERENCES

1. "Solute concentration and inhomogeneous broadening effects on the study of the propagation of the Rayleigh-type optical mixing signal", A.E. Cardenas, J.L. Paz, H.J. Franco and A.J. Hernández. *1st Venezuelan Conference of Chemistry*, Mérida, Venezuela, 1993.
2. "Non-linear spectroscopy applied to the study of electronic transitions on inhomogeneous molecular systems. Concentration effects", A.E. Cardenas, J.L. Paz and A.J. Hernández. *21st International Congress of Theoretical Chemists of Romance Language*. Grenoble, France, 1993.
3. "Absorptive and saturative features in the propagation study of resonant four-wave mixing signals". A.E. Cardenas, J.L. Paz and A.J. Hernández. *43rd Annual Convention of the Venezuelan Association for the Advancement of Science*. Mérida, Venezuela, 1993.
4. "A wavepacket-path integral method for curve crossing problems: Application to resonance Raman spectra and photodissociation cross sections", A.E. Cardenas and R.D. Coalson, *15th International Conference on Raman Spectroscopy*, Pittsburgh, Pennsylvania, 1996.
5. "Calculation of reduced partial cross sections of molecules photodesorbing from a crystal surface at finite temperature: inclusion of curve-crossing effects", A.E. Cardenas and R.D. Coalson, *32nd Midwest Theoretical Chemistry Conference*, Notre Dame, Indiana, 1999.
6. "Molecular dynamics simulations of the folding kinetics of Cytochrome C: The role of non-native contacts", A.E. Cardenas and R. Elber, CIMMS-IPAM Workshop Molecular Modeling and Computation: Perspectives and Challenges, Pasadena, California, November 2003.
7. "Computational study of the folding process of beta sheet proteins: The cold shock family", S. Urahata, A. Clarke, A. Cardenas, American Chemical Society National meeting, Philadelphia 2004.

8. "Computational study of folding pathways of cold shock proteins", S. Urahata, A. Clarke, A.E. Cardenas, American Conference on Theoretical Chemistry, Los Angeles 2005.
9. "Folding mechanisms of cold shock proteins", A.E. Cardenas, S. Urahata, A. Clarke, Biophysical Society Annual Meeting, Salt Lake City 2006.
10. "Effects of mutations on the folding pathways of a cold shock protein", A. Clarke, S. Urahata, A.E. Cardenas, American Chemical Society National meeting, Atlanta, 2006
11. "Computer simulations of the folding process of apomyoglobin", M. Dametto, A.E. Cardenas, American Chemical Society National meeting, San Francisco, 2006.

B. TALKS AT RESEARCH CONFERENCES

1. "Conformational changes and folding pathways of proteins computed using the stochastic difference equation", A.E. Cardenas and R. Elber, American Chemical Society National meeting, New York, September 2003.
2. "Study of mechanisms of protein folding using an algorithm based on the classical action", A.E. Cardenas, International Congress of Theoretical Chemists of Latin Expression, Venezuela, 2005.
3. "Determination of protein folding pathways by optimization of the classical action", A.E. Cardenas, A. Clarke, M. Dametto, American Chemical Society National meeting, San Francisco, September, 2006.

C. INVITED TALKS AT UNIVERSITIES AND INSTITUTES

1. National Institute of Standards and Technology, Biotechnology Division, Gaithersburg, Maryland, 2000.
2. University of South Florida, Quantum Project Group, Gainesville, 2004
3. Florida Annual Meeting and Exposition, Orlando, May 2007
4. University of Pittsburgh, Symposium of molecular and materials modeling at Pitt: Past, Present, and Future, May 2007.

Students Supervised

Postdoctoral researchers:

Dr. Sergio Urahata (2003-2005)

Graduate students:

Adam Clarke (2004-), Mariangela Dametto (2004-), Shawn Hamm (2005-), Christi Young(2006-), Yongxue Yu (2007-)

Undergraduate student:

Simantha Ather, Kenny Aristide, Jimmy Rodriguez, Hai Nguyen

Courses and Committees

A. COURSES TAUGHT

At Simon Bolivar University

General Chemistry I (August 1993-October 1994) Principles and applications of chemistry including properties of substances and reactions, thermochemistry, atomic-molecular structure and bonding, periodic properties of elements and compounds (About 65 students/trimester)

At Cornell University

Bioinformatics Workshop at the Cornell Theory Center (August 2002) Train the participants in the use of molecular simulation techniques (about 25 students)

At USF

CHM 2045 General Chemistry I (Fall 2006)

CHM 3400/4410 (Elementary) Physical Chemistry I (Fall 2004, Fall 2005) A dual section undergraduate course focusing on thermodynamics.

CHM 4412 Physical Chemistry III (Spring 2005, Spring 2007) Topics: Elementary statistical mechanics, kinetics and electrostatics.

CHM 6938 Statistical Mechanics (Spring 2004) An upper level special topics course for graduate students that focuses on the basic principles of statistical mechanics: ensembles, classical and quantum formalisms, phase transitions and liquids (5 students).

CHM 6938 Advanced Quantum Mechanics II (Spring 2006) An upper level course for graduate students. Topics: group theory, atomic and molecular structure and spectra, electronic structure calculations, molecular properties.

CHM 6938 Tools of Research I (Fall 2004, Spring 2006). This graduate course (divided in modules) introduces students to different experimental and computational techniques. I taught part of the computational module.

B. COMMITTEES AND DUTIES

Department-level

Physical Chemistry Division (2003-Present)
Graduate Student Recruitment Committee (2003-Present)
Computer Committee (2003-Present)

College level

Computer Committee (2004-Present)
Steering Committee for Research Computing (2005-Present)

C. GRADUATE THESIS COMMITTEE

Ph.D. candidates from other research groups:

Christine Neipert
Abraham Stern
Hla Win
Ben Roney

Ph.D. candidates from my research group:

Adam Clarke
Mariangela Dametto
Shawn Hamm
Christi Young

D. SERVICE OUTSIDE OF UNIVERSITY

Grant reviewer for the following granting agencies:

National Institutes of Health
National Science Foundation
U.S. Civilian Research and Development Foundation

Reviewer for the following Journals:

Biophysical Journal
Journal of Molecular Structure: THEOCHEM

Professional Memberships

- American Chemical Society
- Biophysical Society
- American Association for the Advancement of Science
- Sigma Xi