

ADRIAN E. ROITBERG
Quantum Theory Project
University of Florida
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(352) 392-6972
adrian@qtp.ufl.edu

EDUCATION

University of Illinois at Chicago.	Chemistry.	PhD.	1992
Universidad de Buenos Aires, Argentina.	Chemistry.	Licenciado	1987

RESEARCH EXPERIENCE

12/03-Present **Associate Professor**, Quantum Theory Project and Department of Chemistry, University of Florida. Computational biophysics. Enhanced sampling techniques.

8/03-12/03 **Associate Scientist**, Quantum Theory Project and Department of Chemistry, University of Florida. Computational biophysics. Enhanced sampling techniques.

1/01-8/03 **Assistant Scientist**, Quantum Theory Project and Department of Chemistry, University of Florida. Computational biophysics. Enhanced sampling techniques.

3/98-12/00 **Affiliate Assistant Professor**. Computational Sciences Institute, George Mason University. Global optimization and properties of atomic and molecular clusters.

1/96-12/00 **Guest Research Scientist**. Biotechnology Division, National Institute of Standards and Technology. Modeling of electron transfer processes, global optimization techniques and mixed quantum/classical protein modeling.

10/92-12/95 **Postdoctoral Fellow**. Chemistry Department, Northwestern University. Quantum vibrational behavior of large systems, particularly biomolecules. Time dependent self consistent field approximation on systems with weak coupling. Molecular electronics. Advisor: Prof. Mark Ratner.

3/94-6/94 **Postdoctoral Fellow** Fritz-Haber Center for Molecular Dynamics, The Hebrew University of Jerusalem, Israel. Vibrational states in proteins. Advisor: Prof. Benny Gerber.

Adrian E. Roitberg

9/89-9/92 **Graduate student.** Chemistry Department. University of Illinois at Chicago. Development of the Locally Enhanced Sampling method for conformational searches in biomolecules. Co-developer of MOIL, a public domain program for general molecular dynamics in biomolecules. Advisor: Prof. Ron Elber.

4/87-9/89 **Graduate researcher.** Department of Inorganic, Analytical and Physical Chemistry, University of Buenos Aires. Argentina. Effect of radiation exposure on inorganic metal complexes.

TEACHING EXPERIENCE

1. CHM3400. Physical Chemistry with Applications to Biology. 38 students. Fall 2004.
2. CHM XXX. Molecular Biophysics. . 15 students. Spring 2004
3. CHM6580. Computational Chemistry. 20 Students. Spring 2004
4. CHM XXX. Molecular Biophysics. . 15 students. Fall 2003
5. CHM 6580. Computational Chemistry. 12 Students, Spring 2003 .
6. CHM 6934. Quantum Theory Project Graduate Seminar. 4 Students. Spring 2002.
7. PHY 6932. Quantum Theory Project Graduate Seminar. 4 Students. Spring 2002.
8. CHM 3400. Physical Chemistry with Applications to Biology. 30 students. Fall 2001.
9. Statistical Thermodynamics (Graduate Course). Lecturer. George Washington University. 4 students. Fall 1996.
10. Quantum Chemistry (Graduate Course). Lecturer. George Washington University. 4 students. Spring 1996.
11. General Chemistry and Physical Chemistry. Teaching Assistant. University of Illinois at Chicago. 1989-1991.
12. Analytical Chemistry and Radiochemistry. Teaching Assistant. Department of Inorganic, Analytical and Physical Chemistry. University of Buenos Aires, Argentina. 1987-1989.
13. Analytical Chemistry. Undergraduate Teaching Assistant. Department of Inorganic, Analytical and Physical Chemistry. University of Buenos Aires. Argentina. 1985.

Adrian E. Roitberg

14. High School chemistry teacher. Technical School O.R.T. Buenos Aires. Argentina. 1983.

STUDENT SUPERVISION

Present:

Hui Xiong (3rd year graduate, Physics)
Ozlem Demir (2nd year graduate, Chemistry)
Giorgios Leonis (2nd year graduate, Chemistry)
Jennifer Mallek (1st year graduate, Chemistry)
Christina Crecca (1st year graduate, Chemistry)
Seonah Kim (1st year graduate, Chemistry)
Robert Abel (4th year undergraduate, Chemistry)
Julio Palma (4th year undergraduate, Chemistry)

Past:

Colin Reese. (summer undergraduate Student, 2002)
Eva (Tina) Rivera. (graduate. 2001-2002)
John Sites III. (undergraduate. 2002)
Amer Hanano. (undergraduate. 2002)
Yi Mao. (graduate, 1995.)
Paul Sack. (undergraduate, 1994)
Amanda Cheong. (undergraduate, 1993)
Todd Wanta. (undergraduate. 1992-1994)

PROFESSIONAL MEMBERSHIPS

1. Member of American Chemical Society (Physical Chemistry Division, theoretical and biophysical chemistry subdivisions).
2. Member of American Physical Society.
3. Member of the American Association for the Advancement of Science.
4. Phi Kappa Phi Honor Society. 1991
5. Sigma Xi Honor Society. 1997

SERVICE

1. Member. External Scientific Advisory Committee. MBRS-SCORE program. University of Puerto Rico. Mayaguez. PR
2. Member. Editorial Board. International Journal of Quantum Chemistry. 2004-

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3. Member. Editorial Board. Advances in Quantum Chemistry. 2004-
4. Co-Organizer of the 45th Sanibel Symposium, St. Augustine, FL, Feb 2005.
5. Guest Editor. Special Issue of "Journal of Molecular Graphics and Modelling" on Conformational Sampling . May 2004
6. Co-Organizer of the 44th Sanibel Symposium, St. Augustine, FL, Feb 2004.
7. Co-Organizer of the 43th Sanibel Symposium, St. Augustine, FL, Feb 2003.
8. Co-Organizer of the 42th Sanibel Symposium, St. Augustine, FL, Feb 2002.
9. Advisor and Reviewer for the "National Science Agency" in Argentina. 2001-Present.
10. Organizer of an ACS symposium and the National American Chemical Society meeting. "Enhanced Sampling Techniques for Monte Carlo and Molecular Dynamics". Orlando, FL. 2002.
11. Member of the NSF review panel for the Supercomputing Alliance Allocations Board. (AAB). 2002-Present.
12. Member of the NSF review panel for the Supercomputing National Resources Allocation Committee. (NRAC). 2002-Present.
13. In charge of Hypercube Scholar's award for 2001/2002/2003.
14. Provided support for visualization and system management at QTP. 2001-2003.
15. Member of the Undergraduate curriculum committee. 2002-2003
16. Co-Organizer of the 41th Sanibel Symposium, St. Augustine, FL, Feb 2001.
17. Ad-Hoc Member of the MDCN2 study section of the National Institutes of Health (2000).
18. Member of the Editorial Board of TMMeC (The Molecular Modeling e-Conference). 1998-2002.
19. Session Chair for the Biophysical Symposium in the 1995 National ACS Meeting in Chicago, IL.
20. Co-organizer for the Midwest Theoretical Conference in May 1995. Northwestern University.
21. Co-organizer for the third international meeting "Youth Building the Future". Buenos Aires. Argentina. 1989.

Adrian E. Roitberg

22. Student Member of the Board of the School of Sciences. University of Buenos Aires. 1985-1987.
23. Graduate Member of the Board of the School of Sciences. University of Buenos Aires. 1987-1989.
24. Reviewer for: The Proceeding of the National Academy of Sciences, The Journal of Chemical Physics, Journal of Molecular Structure, The Journal of Physical Chemistry, The Journal of the American Chemical Society, The Biophysical Journal, The Journal of Inorganic Biochemistry, The Journal of Medicinal Chemistry, Physics Letters, The International Journal of Quantum Chemistry, Advances in Quantum Chemistry, The Internet Journal of Chemistry, Journal of Computational Chemistry, International Journal of Molecular Sciences, Journal Of Raman Spectroscopy, Langmuir, The Petroleum Research Fund of the American Chemical Society, Department of Energy, Basic Energy Sciences, National Science Board, Argentina, City University of New York-FRAP Program, National Science Foundation.

FUNDED PROPOSALS

1. "Molecular wires and nano-wires: properties and control". Department of Energy. Office of Basic Energy Sciences. Nano-Scale Science, Engineering and Technology Program. DE-FG02-02ER45995. Adrian E. Roitberg. Co-P.I. \$750,000, 2002-2005.
2. "Peptide and protein folding: the view from the energy minima." College of Liberal Arts and Sciences Research Award. \$10,900. Adrian E. Roitberg. P.I. 2001.
3. Support for an ACS symposium titled "Enhanced sampling techniques for Monte Carlo and molecular dynamics". Petroleum Research Fund. \$2,400. Adrian E. Roitberg. P.I. 2001.

PUBLICATIONS

1. "Kinetics of internal-Ilop formation in polypeptide chains: a simulation study". Dana Doucet, Adrian E. Roitberg and Steve J. Hagen. Submitted to *Biophys J.* June 2006.
2. "The Catalytic Mechanism of Peptidylglycine α -Hydroxylating Monooxygenase Investigated by Computer Simulation." Alejandro Crespo, Marcelo A. Martí, Adrian E. Roitberg, L. Mario Amzel, and Darío A. Estrin. Accepted *J.Amer.Chem.Soc.* Aug 2006.
3. "Comparison of multiple Amber force fields and development of improved protein backbone parameters". Viktor Hornak, Robert Abel, Asim Okur, Bentley Strockbine, Adrian Roitberg and Carlos Simmerling. Accepted *Proteins: Structure, Function, and Bioinformatics.* June 2006
4. "Structural analysis of ligand binding and catalysis in chorismate lyase". Natasha Smith, Adrian E. Roitberg, Eva Rivera, Andrew Howard, Marcia J. Holden, Martin Mayhew, Salita Kaistha, and D.T. Gallagher. *Archives of Biochemistry and Biophysics* **445**:72-80 (2006)
5. "Theoretical Study of the Isomerization Mechanism of Azobenzene and Disubstituted Azobenzene Derivatives". Christina R. Crecca and Adrian E. Roitberg. *J. Phys. Chem. A.* 110(26); 8188-8203 (2006)
6. "Molecular dynamics simulations of alkanethiol monolayers with azobenzene molecules on the Au (111)." Ping Jiang, Lin-Lin Wang, Adrian E. Roitberg, Jeffrey L. Krause, Hai-Ping Cheng. Submitted to *J. Phys. Chem. B.* October 2005
7. "Free Energy calculations with non-equilibrium methods. Applications of the Jarzynski Relationship". Hui Xiong, Alejandro Cresp, Marcelo Marti, Dario Estrin and Adrian E. Roitberg. *Theoretical Chemistry Accounts.* **106**(1-3): 338-346 (2006)
8. "Energy Transfer in the Nanostar: The Role of Coulombic Coupling and Dynamics". Wilfredo Ortiz, Brent P. Krueger, Valeria D. Kleiman, Jeffrey L. Krause and Adrian E. Roitberg. *J. Phys. Chem. B,* **109**:11512 -11519 (2005)
9. "Non-Equilibrium Approaches to Free Energy Calculations". Adrian E. Roitberg. *Annual Reports in Computational Chemistry.* Chapter 8, page 103. Elsevier (2005)
10. "Multiple-Steering Molecular Dynamics QM-MM Free Energy Profiles in Enzymatic Reactions. Alejandro Crespo, Marcelo A. Martí, Darío A. Estrin, and Adrian E. Roitberg. *J. Am. Chem. Soc.,* **127** (19), 6940 -6941, 2005.
11. "Special issue: Conformational sampling". Adrian E. Roitberg and Carlos L. Simmerling. *Journal of Molecular Graphics and Modelling.* 22:317 (2004)

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12. "Molecular Dynamics of Poly(benzylphenyl ether) Dendrimers: Effects of Backfolding on Förster Energy Transfer Rates". Wilfredo Ortiz, Jeffrey Krause and Adrian E. Roitberg. *Journal of Physical Chemistry B*. 108:8218-8225 (2004)..
13. "Coherent electron transport through an azobenzene molecule: A light driven molecular approach". C. Zhang, M.-H.Du, H.-P.Cheng, X.-G.Zhang, A.E.Roitberg and J.L.Krause. *Phys. Rev. Lett.* 92, 158301 (2004)
14. "A DFT based QM-MM Approach Designed for the Treatment of Large Molecular Systems: Application to Chorismate Mutase". Alejandro Crespo, Damián A. Scherlis, Marcelo A. Martí, Pablo Ordejón, Adrián E. Roitberg, and Darío A. Estrin. *Journal of Physical Chemistry B*, 107 (49), 13728 -13736, 2003.
15. "Kinetic isotope effects in the active site of B.subtilis chorismate mutase" Sharon E. Worthington, Adrian E. Roitberg and Morris Krauss. *International Journal of Quantum Chemistry*, 94: 287-292 (2003)
16. "Smaller and faster: The 20-residue Trp-cage folds in 4 microseconds". Linlin Qiu, Suzette A. Pabit, Adrian E. Roitberg and Stephen J. Hagen. *Journal of the American Chemical Society*, 124:12952-12953 (2002)
17. "4,5-Dehydrooctafluoro[2.2]paracyclophane: facile generation and extraordinary Diels-Alder reactivity", Merle A. Battiste, Jian-Xin Duan, Yi-An Zhai, Ion Ghiviriga, Khalil A. Abboud, Adrian E. Roitberg, G. Robert Shelton and William R. Dolbier, Jr. *Tetrahedron Letters*, 43(39):7047-7049 (2002) .
18. "All atom structure prediction and folding simulations of a stable protein" Carlos L. Simmerling, Bentley Strockbine and Adrian E. Roitberg. *Journal of the American Chemical Society*. 124 (38):11258 –11259 (2002)
19. "Solvent-induced symmetry breaking of nitrate ion in aqueous clusters: A QM/MM study". Mariano C. González Lebrero, Damián E. Bikiel, M. Dolores Elola, Darío A. Estrin and Adrian E. Roitberg. *Journal of Chemical Physics*, 117(6):2718-2722 (2002).
20. "Benzocycloarene hydroxylation by P450 biocatalysis". Martin P. Mayhew, Adrian E. Roitberg, Yadu Tewari, Marcia J. Holden, Dave Vanderah and Vincent L. Vilker. *New Journal of Chemistry*, 26:35-42 (2002).
21. "Strontium clusters: many-body potential, energetics and structural transitions". Guanming Wang, Estela Blaisten-Barojas, Adrian E. Roitberg, and T.P. Martin. *Journal of Chemical Physics*, 115:3640 (2001).
22. "An MD/QM study of the chorismate mutase catalyzed claisen rearrangement reaction". Sharon E. Worthington, Adrian E. Roitberg and Morris Krauss. *Journal of Physical Chemistry B*, 105:7087-7095 (2001).

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23. "Raman and FT-IR spectroscopies of fluorescein in solution". LiLi Wang, Adrian E. Roitberg, Curt Meuse and Adolfas K. Gaigalas. *Spectrochimica Acta A*, 57,1781-91(2001).
24. "The electronic spectrum of the prephenate di-anion. An experimental and theoretical (MD/QM) comparison". Adrian E. Roitberg, Sharon Worthington, Marcia J. Holden, Martin P. Mayhew and Morris Krauss. *Journal of the American Chemical Society* 122:7312-7316,(2000).
25. "Molecular wire conductance: electrostatic potential spatial effects". Vladimiro Mujica, Adrian E. Roitberg and Mark A. Ratner. *Journal of Chemical Physics* 112:6834-6839 (2000).
26. "Pulsed terahertz spectroscopy of biomolecules". Andrea G. Markelz, Adrian E. Roitberg and Edwin H. Heilweill. *Chemical Physics Letters* 320:42-48 (2000).
27. "The injecting energy at molecule/metal interfaces: implications for conductance of molecular junctions from an ab-initio molecular description". Sophia N. Yaliraki, Adrian E. Roitberg, Carlos Gonzalez, Vladimiro Mujica and Mark A. Ratner. *Journal of Chemical Physics* 111:6997-7002 (1999).
28. "Electron transfer in molecules and molecular wires; geometry dependence, coherent transport and control". Vladimiro Mujica, Abraham Nitzan, Yi Mao, William Davis, Mathieu Kemp, Adrian E. Roitberg and Mark A. Ratner. *Advances in Chemical Physics* 107:403-429 (1999).
29. "Molecular wires: charge transport, mechanisms and control". Mark A. Ratner, William Davis, Mathieu Kemp, Vladimiro Mujica, Adrian E. Roitberg and Sophia Yaliraki. *Annals of the New York Academy of Sciences* 852:22-36 (1998).
30. "Binding and electron transfer between putidaredoxin and cytochrome P450cam (CYP101). Theory and experiments". Adrian E. Roitberg, Marcia Holden, Martin Mayhew, Igor Kurnikov, David Beratan and Vincent Vilker. *Journal of the American Chemical Society* 120:8927-8932 (1998).
31. "A molecular dynamics study of Fe₂S₂ putidaredoxin. Multiple conformations of the C-terminal region". Adrian E. Roitberg. *Biophysical Journal* 73:2138-2148 (1997).
32. "Probing the interactions of putidaredoxin with redox partners in camphor P450 5-monooxygenase by mutagenesis of surface residues". Marcia Holden, Martin Mayhew, David Bunk, Adrian E. Roitberg and Vincent Vilker. *Journal of Biological Chemistry*. 272:21720-21725 (1997).
33. "A vibrational eigenfunction for a protein: The anharmonic Coupled-Mode Ground State of BPTI". Adrian E. Roitberg, R. Benny Gerber and Mark A. Ratner. *Journal of Physical Chemistry B*.101: 1700-1706 (1997).

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34. "Molecular wires: resonances, staircases, rectification, bonding and speculation". Mathieu Kemp, Vladimiro Mujica, Adrian E. Roitberg, Yi Mao and Mark A. Ratner. *Atomic and Molecular Wires*, *NATO ASI Series E. Applied Sciences*. 341:203-217. C. Joachim (Ed.). Kluwer Academic Publishers (1997).
35. "Moller-Plesset perturbation theory applied to vibrational problems". Lawrence Norris, Mark A. Ratner, Adrian E. Roitberg and R. Benny Gerber. *Journal of Chemical Physics*. 105:11261-11267 (1996).
36. "Molecular wires, extended couplings and disorder effects". Mathieu Kemp, Adrian E. Roitberg, Todd Wanta, Vladimiro Mujica and Mark A. Ratner. *Journal of Physical Chemistry* 100:8349-8355 (1996).
37. "A model for coulomb interaction in electron transport in one-dimensional mesoscopic devices". Mujica, Vladimiro; Kemp, Mathieu; Roitberg, Adrian; Ratner, Mark. *Condensed Matter Theories* 11:261-272 (1996).
38. "Current-voltage characteristics of molecular wires. Eigenvalue staircase, coulomb blockade and rectification". Vladimiro Mujica, Mathieu Kemp, Adrian E. Roitberg and Mark A. Ratner. *Journal of Chemical Physics* 104:7296 (1996).
39. "Anharmonic wave functions of proteins: quantum self-consistent field calculations of BPT1". Adrian E. Roitberg, Ron Elber, R. Benny Gerber and Mark A. Ratner. *Science* 268, 1319-1322 (1995).
40. "MOIL: a program for simulations of macromolecules". Ron Elber, Adrian E. Roitberg, Carlos L. Simmerling, Robert Goldstein, Hy Li, Gennady Verkhiver, Chen Keasar, J. Zhang and Alex Ulitsky. *Computer Physics Communications*. 91, 159 (1995)
41. "Resonances and interference effects on the effective electronic coupling in electron transfer". Amanda Cheong, Adrian E. Roitberg, Vladimiro Mujica and Mark A. Ratner. *Journal of Photochemistry and Photobiology: A, Chemistry* 82, 81-86 (1994).
42. "A perturbed mean field approach to the decay rates of excited vibrational states in extended systems: an application to $I_2(Ne)_n$ ". Adrian E. Roitberg, R. Benny Gerber and Mark A. Ratner. *Journal of Chemical Physics* 100, 4355-4366 (1994).
43. "MOIL: A molecular dynamics program with emphasis in conformational searches and reaction path calculations". Ron Elber, Adrian E. Roitberg Carlos L. Simmerling, Robert Goldstein, Gennady Verkhivker, Hy Li and Alex Ulistky. *NATO ASI Series B. Physics*. 325:165-191 (1994).
44. "Modeling side-chains in peptides and proteins with the Locally Enhanced Sampling/simulated annealing method". Adrian E. Roitberg and Ron Elber. "The

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Protein Folding Problem and Tertiary Structure Determination". Ed K.Merz Jr. and S. Le Grand. Birkhauser Pub (1994).

45. "Modeling side-chains In peptides and proteins - Application of the locally enhanced sampling and the simulated annealing methods to find minimum energy conformations." Adrian E. Roitberg and Ron Elber. *Journal of Chemical Physics*. 95,9277-9287(1991).
46. "Conformational transitions". Ryzard Czerminski, Adrian E. Roitberg, Chyung Choi, Alex Ulitsky and Ron Elber. AIP 239. *Advances in Biomolecular Simulations* 153-173. (1991).
47. "Reductive dissolution of neutron and gamma irradiated magnetite". Maria dos Santos Afonso, Cecilia Di Risio, Adrian E. Roitberg, Roberto Marqués and Miguel Blesa. *International Journal of Applied Instrumentation Part. C. Radiation in Physics and Chemistry*. 36:3 (1990).

PRESENTATIONS

1. Invited Talk. "Uses of molecular dynamics in structural and Unstructural Biology". University of South Florida. Tampa, FL. April 2006.
2. Invited talk on "FRET: recalibrating the molecular ruler". Florida State University. Tallahassee, FL. April 2006
3. Invited Talk. "Eppur si muove. Molecular dynamics in structural biology". Biochemistry Department. Washington University at St Louis. St. Louis, MO. October 2005
4. Invited Talk. "Distributed computations for biomolecular structure, dynamics and folding". National meeting of the American Chemical Society. Washington, DC. August 2005.
5. Invited Talk. "Influence of Structure and Dynamics on Energy Transfer Rate sin Dendrimers". Excited State Processes in Nano and Biomolecular Systems. Santa Fe. New Mexico. August 2005
6. Invited Talk. "Eppur si muove. Molecular dynamics in structural biology". Fifth Annual Mercury Conference. Hamilton College. Clinton, NY. July 2005
7. Invited talk on "Uses of Molecular Dynamics in Structural Biology". University of Puerto Rico. San Juan Puerto Rico. February 2005.

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8. Invited talk on "FRET: recalibrating the molecular ruler". University of Florida. October 2004
9. Invited talk on "Equilibrium Free Energies via Non-Equilibrium Thermodynamics". University of Florida. FL. October 2004.
10. Invited talk on "QM/MM methods for enzyme environments". Joint University of Pittsburgh/Carnegie Mellon University. Pittsburgh, PA. September 2004.
11. Invited talk on "QM/MM methods for enzyme environments". National ACS meeting. Philadelphia. PA. August 2004
12. Invited talk on "Energy Transfer in Dendrimeric Systems". Los Alamos National Laboratory. Los Alamos, NM. June 2004
13. Invited talk on "Energy Transfer in Dendrimeric Systems". University of New Mexico, Albuquerque, NM. June 2004
14. Invited talk on "Uses of Molecular Dynamics in Structural Biology" Instituto de Investigaciones Bioquimicas, Buenos Aires, Argentina, March 2004
15. Invited talk on "Protein Folding and Structure Prediction: Are we there yet?". Instituto de Biotecnologia de Rosario. Rosario, Argentina, March 2004
16. Talk on "On Lizzard's Spit, Brackish Order and Protein Folding". Florida International University. Miami, FL. January 2004
17. Talk on "Molecular Dynamics for Protein Folding". Michigan Technological University. Houghton, MI. December 2003.
18. Talk on "On Lizzard's Spit, Brackish Order and Protein Folding". University of Chicago. Chicago, IL. November 2003.
19. Talk on "On Lizzard's Spit, Brackish Order and Protein Folding". University of Florida, September 2003.
20. Invited talk on "Miniproteins and Fast Folders". CECAM workshop. Lyon, France. September 2003
21. Invited talk on "Protein Folding". Universidad de Barcelona. Barcelona, Spain. September 2003
22. Invited talk on "Protein Folding and Structure Prediction: Are we there yet?". Universidad de Buenos Aires, Argentina, July 2003

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23. Invited talk on "Protein Folding and Structure Prediction: Are we there yet?". Instituto de Investigaciones Bioquímicas, Argentina, July 2003
24. Invited talk on "Protein Folding and Structure Prediction: Are we there yet?". Emory University. Atlanta, GA. March 2003
25. Invited talk on "Peptide and Protein Folding and Structure Prediction". Texas Tech. University. Lubbock, TX, October 2002
26. Invited talk on "Peptide and Protein Folding and Structure Prediction". University of Maryland Baltimore County. Baltimore, MD. September 2002
27. Contributed talk on "Peptide folding: many routes to the native state". Annual American Physical Society March Meeting. Indianapolis. March 2002.
28. Invited talk on "Peptide folding: many routes to the native state". 3rd international Congress in Chemistry: Rediscovering the Science. Monterrey, Mexico. March 2002.
29. Invited talk on "An MD/QM investigation of the chorismate mutase catalyzed Claisen rearrangement". 4th Seminar of Advanced Studies on Molecular Design and Bioinformatics. Havana, Cuba. February 2002.
30. Invited talk on "Peptide folding: many routes to the native state". 4th Seminars of Advanced Studies on Molecular Design and Bioinformatics. Havana, Cuba. February 2002.
31. Contributed talk on "Computational Studies of channel function in glutamine-dependent amidotransferases". Xiang Wang, Adrian E. Roitberg and Nigel Richards. 42th Sanibel Symposium. February 2002.
32. Contributed poster on "Structural studies of poly(benzylphenyl ether) dendrimers using molecular dynamics techniques". Wilfredo Ortiz, Adrian E. Roitberg and Jeffrey L. Krause. 42th Sanibel Symposium. February 2002.
33. Contributed poster on "Ligand escape from Chorismate Lyase". Eva Rivera and Adrian E. Roitberg. 42th Sanibel Symposium. February 2002.
34. Contributed poster on "Solvent-induced symmetry breaking of nitrate ion in aqueous clusters: A QM/MM study". Mariano C. González Lebrero, Damián E. Bikiel, M. Dolores Elola, Darío A. Estrin and Adrian E. Roitberg. 42th Sanibel Symposium. February 2002.

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35. Invited talk on "An MD/QM investigation of the chorismate mutase catalyzed Claisen rearrangement". Jackson State University. Jackson MS. December 2001.
36. Invited talk on "Peptide folding: many routes to the native state". Indiana University. Bloomington, IN. October 2001.
37. Invited talk on "An MD/QM investigation of the chorismate mutase catalyzed Claisen rearrangement". Indiana University. Bloomington, IN. October 2001.
38. Invited talk on "Peptide folding: many routes to the native state". Florida State University. Tallahassee, FL. October 2001.
39. Invited talk on "An MD/QM investigation of the chorismate mutase catalyzed Claisen rearrangement". Florida State University. Tallahassee, FL. October 2001.
40. Contributed talk on "Peptide folding: many routes to the native state." Panamerican Workshop on Molecular and Materials. Sciences: Theoretical and Computational Aspects. Gainesville, FL. February 2001.
41. Contributed poster on "Conformational preferences for two neuropeptides". Eva Rivera and Adrian Roitberg. Florida Section of ACS. March 2001.
42. Contributed talk on "Peptide folding: many routes to the native state". Biocomputing 2001. Gainesville, FL. February 2001.
43. Invited talk on "An MD/QM investigation of the chorismate mutase catalyzed Claisen rearrangement". George Mason University. Fairfax, VA. November 2000
44. Contributed talk on "MD/QM study of the chorismate mutase catalyzed Claisen rearrangement reaction". Adrian E. Roitberg, Sharon E. Worthington and Morris Krauss. National Meeting of the American Chemical Society. Washington, DC, August 2000.
45. Invited talk on "Genetic algorithms as global optimizers in peptides and clusters". Department of Physics. State University of New York at Buffalo. Buffalo, NY. March 2001.
46. Invited talk on "An MD/QM investigation of the chorismate mutase catalyzed Claisen rearrangement". Quantum Theory Project. University of Florida, Gainesville. February 2000.
47. Invited talk on "Binding and electron transfer between putidaredoxin and cytochrome P450cam". 11th international conference on cytochrome P450: Biochemistry, Biophysics and Molecular Biology. Sendai, Japan. August 1999.

48. Invited talk on "The electronic spectrum of prephenate, theory and experiments". Chemistry Department, SUNY at Stony Brook. July 1999.
49. Invited talk on "Binding and electron transfer in the putidaredoxin-cytochrome P450cam complex". University of Buenos Aires, Argentina. November 1998.
50. Invited talk on "Genetic algorithms as applied to peptides and clusters". University of Quilmes, Argentina. November 1998.
51. Invited talk on "Molecular wires". University of Quilmes, Argentina. November 1998.
52. Invited talk on "Computation of the conductance decay length in molecular wires". 215th National Meeting of the American Society Meeting, Dallas, TX. April 1998.
53. Contributed poster on "Binding and electron transfer between putidaredoxin and cytochrome P450cam (CYP101). Theory and experiments". Adrian Roitberg, Marcia Holden, Martin Mayhew, Igor Kurnikov, David Beratan and Vincent Vilker. 215th National Meeting of the American Chemical Society. Dallas, TX, April 1998.
54. Invited talk on "Genetic algorithms as applied to peptides and clusters". George Mason University, Fairfax, VA. March 1998.
55. Invited talk on "Binding and electron transfer in the putidaredoxin-cytochrome P450cam complex". Northwestern University, Evanston, IL. September 1997.
56. Invited talk on "Theoretical protein spectroscopy for multiple minima". University of Chicago, Chicago, IL. September 1997.
57. Invited talk on "Theoretical protein spectroscopy for multiple minima". George Mason University, Fairfax, VA. September 1997.
58. Contributed poster on "Modeling the interactions between Putidaredoxin and Cytochrome P450cam". Adrian Roitberg. Biological Electron Transfer Chains. NATO/ESF advanced workshop. Tomar, Portugal. May 1997
59. Invited talk on "Binding and electron transfer in the putidaredoxin-cytochrome P450cam complex". University of California San Francisco, San Francisco, CA. April 1997
60. Contributed poster on "Modeling the interactions between Putidaredoxin and Cytochrome P450cam". Adrian Roitberg. 213th National Meeting of the American Chemical Society. San Francisco, CA. April 1997.

61. Invited talk on "Binding and electron transfer in a protein complex". University of Iowa, Iowa City, IA. March 1997.
62. Invited talk on "Introduction to molecular wires and molecular devices". University of Pittsburgh, Pittsburgh, PA. January 1997.
63. Invited talk on "Introduction to molecular wires and molecular devices". American University. Washington, DC. December 1996.
64. Contributed poster on "Role of multiple minima in protein vibrational spectroscopy. Anharmonic eigenfunctions for different conformers". Adrian Roitberg, Ron Elber, R. Benny Gerber and Mark A. Ratner. 212th National Meeting of the American Chemical Society. Orlando, FL. Aug 1996.
65. Contributed poster on "A Molecular dynamics study of putidaredoxin". Adrian E. Roitberg. 212th National Meeting of the American Chemical Society. Orlando, FL. Aug 1996.
66. Invited talk on "Theoretical protein spectroscopy for multiple minima". National Cancer Institute. Frederick, MD. April 1996.
67. Invited talk on "Theoretical protein spectroscopy for multiple minima". National Institute for Standards and Technology. Gaithersburg, MD. April 1996.
68. Contributed poster on "Role of multiple minima in protein vibrational spectroscopy. Anharmonic eigenfunctions for different conformers". Adrian Roitberg, Ron Elber, R. Benny Gerber and Mark A. Ratner. American Conference in Theoretical Chemistry. Park City, UT. 1996.
69. Contributed poster on "A Molecular dynamics study of putidaredoxin". Adrian E. Roitberg, American Conference in Theoretical Chemistry. Park City, UT. 1996.
70. Contributed poster on "Role of multiple minima in protein vibrational spectroscopy. Anharmonic eigenfunctions for different conformers". Adrian E. Roitberg, Ron Elber, R. Benny Gerber and Mark A. Ratner. 1996 Gordon Conference in Theoretical Chemistry. New Hampton, NH. 1996.
71. Contributed poster on "A molecular dynamics study of putidaredoxin." Adrian Roitberg, 1996 Gordon Conference in Theoretical Chemistry. New Hampton, NH. 1996.
72. Invited talk on "Anharmonic vibrational wavefunctions in proteins". Northern Illinois University. Dekalb, IL. October 1995.

73. Invited talk on "Anharmonic vibrational wavefunctions in proteins". University of Wisconsin at Madison. Madison, WI. September 1995.
74. Invited talk on "Anharmonic vibrational wavefunctions in proteins". Ohio State University. Columbus, OH. September 1995.
75. Invited talk on "Anharmonic vibrational wavefunctions in proteins". University of Illinois at Chicago. Chicago, IL. August 1995.
76. Invited talk on "Anharmonic vibrational wavefunctions in proteins". National Institute for Standards and Technology. Gaithersburg, MD. June 1995.
77. Invited talk on "Anharmonic vibrational wavefunctions in proteins". Northwestern University. Evanston, IL. May 1995.
78. Invited talk on "Anharmonic vibrational wavefunctions in proteins". Northwestern University. Evanston, IL. March 1995.
79. Contributed poster on "Vibrational eigenfunction for a protein. The anharmonic coupled-mode ground state of BPTI". Adrian E. Roitberg, Mark A. Ratner, Ron Elber and R. Benny Gerber. 210th National Meeting of the American Chemical Society. Chicago, IL. 1995.
80. Contributed poster on "Vibrational eigenfunction for a protein. The anharmonic coupled-mode ground state of BPTI". Adrian E. Roitberg, Mark A. Ratner, Ron Elber and R. Benny Gerber. 12th Canadian Symposium in Theoretical Chemistry. Fredericton, NB, Canada. 1995.
81. Contributed poster on "Anharmonic wavefunctions in proteins". Adrian E. Roitberg, Mark A. Ratner, Ron Elber and R. Benny Gerber. 28th Midwest Theoretical Chemistry Conference. Evanston, IL. 1995.
82. Contributed poster on "Wet proteins and vibrational states. Beyond normal modes". Adrian E. Roitberg, Mark A. Ratner, Ron Elber and R. Benny Gerber. Workshop on algorithms for macromolecular modeling. Lawrence, KS. 1994.
83. Invited talk on "Anharmonic vibrational wavefunctions in proteins". Institute for the Physics of Liquids and Biological Systems. La Plata. Argentina. December 1994.
84. Invited talk on "Anharmonic vibrational wavefunctions in proteins". University of Notre Dame. South Bend, Indiana.

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85. Contributed poster on "Wet proteins and vibrational states. Beyond normal modes". Adrian E. Roitberg, Mark A. Ratner, Ron Elber and R. Benny Gerber. 208th National meeting of the American Chemical Society. Washington, D.C. 1994.
86. Contributed poster on "Wet proteins and vibrational states. Beyond normal modes". Adrian E. Roitberg, Mark A. Ratner, Ron Elber and R. Benny Gerber. Gordon conference in Computational Chemistry. New Hampton School, NH. 1994.
87. Contributed poster on "A perturbation theory for decay rates of static mean field states: a correlation function formalism". Adrian E. Roitberg, R. Benny Gerber and Mark A. Ratner. 206th National meeting of the American Chemical Society. Chicago, IL. 1993.
88. Contributed poster on "A perturbation theory for decay rates of static mean field states: a correlation function formalism". Adrian E. Roitberg, R. Benny Gerber and Mark A. Ratner. 26th Midwest theoretical chemistry conference. Carbondale, IL. 1993.
89. Contributed poster on "Modeling side-chains in proteins with the LES/SA method: the core of carboxymyoglobin". Adrian E. Roitberg and Ron Elber. Workshop in high performance computing in chemistry. National Institutes of Health. Bethesda. MD, 1993.
90. Contributed poster on "A new approach for enhanced sampling of sidechain conformations in peptides and proteins: Application of the Locally Enhanced Sampling (LES)/simulated annealing method". Adrian E. Roitberg and Ron Elber. Seventh conversation in Biomolecular Stereodynamics. SUNY at Albany. Albany, NY. 1991.
91. Contributed poster on "Enhanced sampling of sidechain conformations of peptides and proteins: A combined LES/SA method". Adrian E. Roitberg and Ron Elber. 1991 Joint regional Central-Great Lakes regional ACS meeting. Indiana University-Purdue University at Indianapolis. IN. 1991.
92. Contributed poster on "A New approach for enhanced sampling of sidechain conformations in peptides and proteins: Application of the Locally Enhanced Sampling (LES)/simulated annealing method". Adrian E. Roitberg and Ron Elber. 24th Midwest theoretical chemistry conference. Northern Illinois University. Dekalb. IL 1991.
93. Contributed poster on "Induced damage by nuclear reactor irradiation of $[\text{Fe}(\text{bipy})_3](\text{ClO}_4)_2$ and its thermal annealing". Adrian E. Roitberg and Cecilia Di Risio and Roberto Marques. VI National Conference in Physical Chemistry. Rio Hondo. Argentina. 1989.

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