ROBERT Q. TOPPER

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CURRENT RESEARCH ACTIVITY

Theoretical chemistry and chemical physics. Statistical mechanics; reaction rate theory; stochastic process algorithms for quantum and classical statistics, including quantum and classical Monte Carlo methods. Machine learning methods for free energy surfaces of biomolecules and materials.

Nanoclusters and atmospheric chemistry. Thermodynamic, spectral and structural properties of nanoclusters of ammonium salts formed via homogenous nucleation in polluted marine environments.

Computational chemistry. Applications of advanced density functional theory and *ab initio* quantum chemistry methods. Quantum studies of solvent and substituent effects on regioselectivity; models of intermolecular forces within molten materials and disordered solids; structures, spectra and bonding trends of organometallic complexes; prediction and characterization of distortions caused by chemical modification of DNA.

PROFESSIONAL EMPLOYMENT SUMMARY

01/2017 – Present	Visiting Research Professor, Department of Chemistry, New York University.
07/2009 – Present	Professor of Chemistry, Cooper Union. Tenured in 2009.
2003 – 2009	Chair and Associate Professor, Department of Chemistry, Medical Technology and Physics, Monmouth University (NJ). Tenured in 2003.
1999 – 2003	Associate Professor of Chemistry, Cooper Union. Tenured in 1999.
1993 – 1999	Assistant Professor of Chemistry, Cooper Union.
1992 – 1993	Postdoctoral Research Associate, Department of Chemistry, University of Rhode Island.
1990 – 1992	Postdoctoral Research Fellow, Department of Chemistry and Minnesota Supercomputer Institute, University of Minnesota.
1986 – 1990	Graduate Teaching Assistant, Department of Chemistry, Yale University.
1983 – 1986	Instructor, Tutor and Computer-Aided Instruction Coordinator, Department of Mathematics, Florida State University and Tallahassee Community College.
1983 – 1985	Undergraduate Research Assistant, Department of Chemistry, Florida State University.

EDUCATION

Ph.D.	Theoretical Physical Chemistry, Yale University (**1990**). *The Dynamics and Kinetics of Reactive Motion Between Multiple Geometric Conformers*.
M.S., M.Phil.	Physical Chemistry, Yale University (**1989**).
B.S.	Physics and Chemistry, Florida State University (**1986**); Honors in Liberal Arts (**1982**).

PROFESSIONAL ORGANIZATIONS

Alpha Chi Sigma, American Chemical Society (NY Section), Order of the Engineer, Phi Lambda Upsilon, Sigma Pi Sigma.

HONORS , FELLOWSHIPS AND AWARDS

Cooper Union Engineering Student Council Student's List (**2010** and **2012**); Phi Lambda Upsilon (**2008**); Minnesota Supercomputing Institute Postdoctoral Research Fellow (**1990-1992**); Kent Graduate Fellowship in Chemistry Award (**1989-1990**); Robert B. Flint Graduate Fellowship in Chemistry Award (**1986–1990**); Florida State University College of Arts and Sciences Leadership Award (**1986**); American Institute of Chemists Senior Award in Chemistry (**1986**); Charles A. Brautlecht and Louise I. Brautlecht Scholarship in Chemistry (**1985-1986**); Sigma Pi Sigma (**1985**); National Merit Scholarship Award (**1981-1985**).

RESEARCH PUBLICATIONS (*=undergraduate coauthor, **=high school student coauthor)

1. E. Schneider, L. Dai**, R.Q. Topper, C. Drechsel-Grau, M.E. Tuckerman, *Stochastic neural network approach for learning high-dimensional free energy surfaces*, ***Physical Review Letters*, 119, p.**150601 (**2017**).
2. J.J. Biswakarma,* V. Ciocoi,* R.Q. Topper, *Energetics, thermodynamics and hydrogen bonding diversity in ammonium halide clusters*, ***Journal of Physical Chemistry A,* 120**(40), pp. 7924-7934 (**2016**).

3. R.Q. Topper, W. V. Feldmann,* D. Bergin,* P.R. Sweeney,* *Simulated annealing and density functional theory calculations of structural and energetic properties of the ammonium chloride clusters $(NH_4Cl)_n$, $(NH_4^+)(NH_4Cl)_n$, and $(Cl^-)(NH_4Cl)_n$, n = 1–13,* ***Journal of Physical Chemistry A***, **115**(38), pp. 10423-10432 **(2011)**.
4. S. Ling, R.Q. Topper, invited book chapter, *On the zero point energy difficulty of quasiclassical trajectory simulations*, in ***Handbook of Computational Chemistry Research***, C. T. Collett and C. D. Robson, Eds., Nova Science Publishers, Hauppauge, NY, pp. 467-476 **(2010).** ISBN: 978-1-60741-047-8 .
5. T.A. Isgro, N. Mathew,** R.Q. Topper, *Structural characterization of N-acetyl-2-aminofluorene adducts to guanine and deoxyguanosine via a molecular mechanics, semi-empirical and density-functional theory cascade method,* ***Journal of Molecular Structure (THEOCHEM)*** **710,** pp.31-43 **(2004).**
6. R.Q. Topper, D.L. Freeman, D. Bergin, K. LaMarche*, *Computational techniques and strategies for Monte Carlo thermodynamic calculations with applications to nanoclusters,* invited book chapter, ***Reviews in Computational Chemistry***, **Vol. 19**, pp. 1-41, K.B. Lipkowitz, R. Larter and T.R. Cundari, Eds., Wiley-VCH/John Wiley and Sons, New York **(2003)**. ISBN 0-471-23585-7.
7. R.Q. Topper, K. Chung*, C. Boelke*, D. Louie*, J.S. Kang*, R. Hannan*, T. Kiang,* L.H. Chan*, *Computational structural determination and energy landscape analysis of the hepatic carcinogen 2-(acetylamino)fluorene,* ***Theoretical Chemistry Accounts*** **109/4**, 233 **(2003).**
8. J. Kritzer*, A. Deaconescu*, J. de la Parra Jr.*, D. Coluccio*, S. Mikhail,* R.Q. Topper, *Benchmarking potential energy models against bulk properties for simulations of bismuth clusters,* ***Internet Journal of Chemistry*** **3**, 12 **(2000)**.
9. R.Q. Topper, *Adaptive path-integral Monte Carlo methods for accurate computation of molecular thermodynamic properties*, invited book chapter, Monte Carlo Methods in Chemical Physics, ***Advances in Chemical Physics*** **105**, Chapter 5, pp. 117-170, D. Ferguson, I. Siepmann, and D.G. Truhlar, Eds., John Wiley & Sons, Inc., New York **(1999)**.
10. F.M. Torres*, E. Agichtein*, L. Grinberg*, G. Yu*, R.Q. Topper, *A note on the application of the "Boltzmann simplex"-simulated annealing algorithm to global optimizations of argon and water clusters,* ***Journal of Molecular Structure (THEOCHEM)*** **419**, 85 **(1997)**.
11. R.Q. Topper, *Visualizing molecular phase space: Non–statistical effects in reaction dynamics,* invited article, in ***Reviews in Computational Chemistry*** **10**, pp. 101-176, K.B. Lipkowitz and D.B. Boyd, Eds., VCH Publishers, New York **(1997)**.
12. A. Matro, D.L. Freeman, R.Q. Topper, *Computational study of the structures and thermodynamic properties of ammonium chloride clusters using a parallel J-walking approach,* ***Journal of Chemical Physics*** 104, 8690 **(1996)**.
13. R.Q. Topper, D.L. Freeman, *Monte Carlo studies of the orientational order-disorder phase transition in solid ammonium chloride, Los Alamos Chemical Physics Preprint Database*, #9403002 **(1994)**. This article was not peer-reviewed but is widely disseminated and has been cited in the primary literature.
14. R.Q. Topper, Q. Zhang, Y.-P. Liu, D.G. Truhlar, *Quantum steam tables. Free energy calculations for* H_2O,D_2O, H_2S, *and* H_2Se *by adaptively optimized Fourier path integrals,* ***Journal of Chemical Physics*** **98**, 4991 **(1993)**.
15. R.Q. Topper, G.J. Tawa, D.G. Truhlar, *Quantum free-energy calculations: A three-dimensional test case,* ***Journal of Chemical Physics*** **97**, 3648 **(1992)**.
16. R.Q. Topper, D.G. Truhlar, *Quantum free-energy calculations: Optimized Fourier path-integral Monte Carlo computation of coupled vibrational partition functions,* ***Journal of Chemical Physics*** **97**, 3648 **(1992)**.
17. N. De Leon, M.A. Mehta, R.Q. Topper, *Cylindrical manifolds in phase space as mediators of chemical reaction dynamics and kinetics II. Numerical considerations and applications to molecular models with two degrees of freedom,* ***Journal of Chemical Physics*** **94**, 8329 **(1991)**.
18. N. De Leon, M.A. Mehta, R.Q. Topper, *Cylindrical manifolds in phase space as mediators of chemical reaction dynamics and kinetics I. Theory,* ***Journal of Chemical Physics*** **94**, 8310 **(1991)**.

EDUCATIONAL MATERIALS AND REVIEWS

1. R.Q. Topper, C.R. Spray, J. Duncan, L.J. Treadwell, S.G. Sobel, *How Many Atoms Are In A Nanowire?,* ***http://www.ionicviper.org*** **(2013).** Contributed learning object (PR)
2. J. Duncan, C.R. Spray, L.J. Treadwell, R.Q. Topper, S.G. Sobel, *Solid State, Semiconductors, Electrochemistry, and Nanowires for Solar Cells: Discuss!* ***http://www.ionicviper.org*** **(2013).** Contributed learning object (PR).
3. R.Q. Topper, *Trends in Measured Redox Potentials and Computed Molecular Orbital Energies of Derivatized Buckminsterfullerene,* ***http://www.ionicviper.org*** **(2013).** Contributed learning object (PR).
4. R.Q. Topper, invited book review of *"Atomistic Approaches in Modern Biology: From Quantum Chemistry to Molecular Simulations. Topics in Current Chemistry, Volume 268,"* ***Journal of the American Chemical Society,*** **129**(31), pp 9830 – 9831 **(2007)** (PR).
5. R.Q. Topper, invited book review of *"Reviews in Computational Chemistry, Vol. 13,"* ***Journal of the American Chemical Society,*** **122**(19), 4845 **(2000)** (PR).
6. *R.Q. Topper, invited book review of "Mathematica Computer Programs for Physical Chemistry,"* ***Theoretical Chemistry Accounts,*** **101**, 439 **(1999)** (PR).

7. *R.Q. Topper, invited book review, "Quantum Mechanics Simulations: Consortium for Upper-level Physics Software by J.R Hiller, I.D. Johnston and D.F. Styer,"* ***Computer Physics Communications,*** **94**,272 **(1995)** (PR).

PRESENTATIONS AND CONFERENCE PROCEEDINGS (presenters' names underlined)

1. *Molecular Modeling of Nanoparticles and Polypeptides*, R.Q. Topper, Department of Chemistry, University of Rhode Island **(2017)**. **Invited lecture.**
2. *Unusual hydrogen bond diversity in ammonium halide nanoclusters*, R.Q. Topper, J.J. Biswakarma,* 57^{h} Sanibel Symposium, University of Florida Quantum Theory Project, St. Simons Island, GA **(2017)**. **Contributed lecture.** (PR)
3. *Computational and theoretical physical chemistry: Applications to ammonium halide nanoclusters*, R.Q. Topper, High Technology High School, Lincroft, NJ **(2017)**. **Invited lecture.**
4. *Mag-walking Monte Carlo and density functional theory calculations of interaction energies in ammonium halide clusters*, R.Q. Topper, J.J. Biswakarma,* V. Ciocoi,* 44th Middle Atlantic Regional Meeting (MARM) of the American Chemical Society, Riverdale, NY **(2016)**. **Contributed lecture.** (PR)
5. *Relative proton acidities within a bicyclic thioacetal*, B. Lee, R.Q. Topper, 63rd Annual Undergraduate Research Symposium, New York section of the American Chemical Society, Queensborough NY **(2015)**. **Contributed lecture.**
6. *Computational studies of structural diversity in nanoparticles of the ammonium halides*, R.Q. Topper, Queensborough Community College, Department of Chemistry, Bayside, NY (**2014**). **Invited lecture.**
7. *Density functional theory study of small Group IV tetrakis(dimethyl)amide clusters*, N. Rao, C. Bock, C.A. Smith, R.Q. Topper, 248th meeting of the American Chemical Society, San Francisco, CA (**2014**). **Contributed poster.** (PR)
8. *Solvent effects on neurotransmitter conformations*, S. Sharif and R.Q. Topper, 62nd Annual Undergraduate Research Symposium, New York section of the American Chemical Society, Queens, NY (**2014**). **Contributed lecture.**
9. *A computational study of the structure of tetrakisdiethylamidozirconium*, A. Grofe, N. Rao, R.Q. Topper, C.A. Smith, Sigma Xi Research Symposium, Saint Joseph University, Philadelphia, PA (**2012**). **Contributed poster.**
10. *Structures, spectra, reaction energies and oxidation trends of NH_4Cl nanocrystallites*, R.Q. Topper, W.V. Feldmann,* I. Markus,* 240th national meeting of the American Chemical Society, Boston, MA (**2010**). **Contributed poster.** (PR)
11. *Computational determination of energy landscapes and conformer distributions of chemically damaged deoxyguanosines*, R.Q. Topper, J.E. Brown,* M. Khalil*, 236th national meeting of the ACS, Philadelphia, PA (**2008**). **Contributed poster.** (PR)
12. R.Q. Topper, O. Dmitrenko, Eds., *Abstracts of the 11th Electronic Computational Chemistry Conference, http://stores.lulu.com/eccc* (**2008**). **Conference abstracts** (all abstracts were peer-reviewed). (PR)
13. R.Q. Topper, G. Sun, Eds., *Proceedings of the 10th Electronic Computational Chemistry Conference,* ***Theoretical Chemistry Accounts*** **117(2) (2007)**; R.Q. Topper and G. Sun, *Introduction to the Proceedings of the 10th Electronic Computational Chemistry Conference,* ***Theoretical Chemistry Accounts*** **117(2),** p. 183 **(2007)**. (PR)
14. *Strategies for Engaging, Leading, and Supporting Undergraduate and High School Students in Computational and Theoretical Chemistry Research Projects*, joint session of the Chemical Education and Physical Chemistry divisions, 230th national American Chemical Society meeting, R.Q. Topper, Washington, D.C. (**2005**). **Invited lecture.** (PR)
15. *Structural and thermodynamic properties of ammonium chloride clusters,* R.Q. Topper, G. Lee,** C. Russamano,* J. Mueller*, 230th national meeting of the ACS, Washington DC (**2005**). **Contributed poster.** (PR)
16. *Structural properties of ammonium chloride clusters,* C. Russamano,* R.Q. Topper**,** Second Annual SURF Symposium, Merck Inc,. Rahway, NJ (**2005**). **Invited poster.**
17. *Modeling DNA Damage: Computational Cascade Analyses of N-Acetyl-2-Aminofluorene (AAF) Adducts to Guanine and Deoxyguanosine*, R.Q. Topper, Symposium on Computational Chemical Dynamics, University of Minnesota, Department of Chemistry and Minnesota Supercomputer Institute (**2004**). **Invited lecture.**
18. R.Q. Topper, O. Dmitrenko, Eds., *Proceedings of the 9th Electronic Computational Chemistry Conference*, ***International Journal of Molecular Sciences*** **Vols. 5-7 (2004);** R.Q. Topper and O. Dmitrenko, *Introduction to the Proceedings of the 9th Electronic Computational Chemistry Conference*, ***International Journal of Molecular Sciences*** **Vol. 5 (2004).** (PR)
19. *Computational modeling of deoxyguanosine adducts*, N. Jain,* R.Q. Topper**,** First Annual SURF Symposium, Merck Inc., Rahway, NJ **(2004)**. **Invited poster.**
20. *Computational modeling of deoxyguanosine adducts,* R.Q. Topper, T. Isgro, N. Mathew**, N. Jain,* N.P. Dayal** **,** 228th national meeting of the ACS, Philadelphia, PA **(2004)**. **Contributed poster.** (PR)
21. *Structural characterization of N-acetyl-2-aminofluorene (AAF) guanine and deoxyguanosine adducts via a molecular mechanics, semi-empirical, and density functional theory cascade method*, T.A. Isgro, N. Mathew,** R.Q. Topper, "Frontiers in DNA Research: An Interdisciplinary Symposium" program at the 226th national meeting of the ACS, New York, NY **(2003). Contributed lecture.** (PR)
22. R.Q. Topper**,** T.A. Isgro, N. Mathew**, *Computational Modeling of Covalent Deoxyguanosine Adducts,*

Abstract of presentation in the "Frontiers in DNA Research: An Interdisciplinary Symposium" program at the 226th national meeting of the ACS, New York, NY **(2003).** Published in ***Chemical Research in Toxicology*** **17(12)**; 1757-1783 **(2004)**. Dedon, P. C.; Penning, T. M., eds. (PR)

23. R.Q. Topper, W.M.F. Fabian, Eds., *Proceedings of the 8th Electronic Computational Chemistry Conference*, special issue, ***Theoretical Chemistry Accounts*** **109/4 (2003);** R.Q. Topper, W.M.F. Fabian, *Introduction to the Proceedings of the 8th Electronic Computational Chemistry Conference*, *Theoretical Chemistry Accounts* **109/4, p.1 (2003).** (PR)
24. *Structural determination and energy landscape analysis of 2-(-acetylamino)fluorene,* R.Q. Topper, K. Chung,* C. Boelke,* D. Louie,* J.S. Kang,* R. Hannan,* T. Kiang,* L.H. Chan,* American Conference on Theoretical Chemistry **(2002). Contributed poster.** (PR)
25. *Structural determination of 2-(-acetylamino)fluorene,* R.Q. Topper, K. Chung,* C. Boelke,* D. Louie,* J.S. Kang,* R. Hannan,* T. Kiang,* L.H. Chan,* Eighth Electronic Computational Chemistry Conference **(2002). Contributed presentation.** (PR)
26. *Monte Carlo Quantum Thermodynamics of Really Hot Molecules*, R.Q. Topper, University of Memphis, Department of Chemistry (**2001**). **Invited lecture.**
27. *Quantum Rovibrational Thermodynamics of Really Hot Molecules Using Adaptive Fourier Path-Integral Monte Carlo Methods,* R.Q. Topper, D. Bergin*, C. Briscoe*, T. Isgro*, J. Kirtland*, D.G. Truhlar, S.L. Mielke, Y.-P. Liu, 220th national meeting of the ACS, Washington, DC. **(2000). Contributed lecture.** (PR)
28. *Analysis of the Accuracy Achieved by Adaptive Fourier Path-Integral Monte Carlo Thermodynamic Computations in the Combustion Regime,* T. Isgro*, J. Kirtland*, C. Briscoe*, R.Q. Topper, 220th national meeting of the American Chemical Society, Washington, DC. **(2000). Contributed poster.** (PR)
29. *Benchmarking Potential Energy Models Against Bulk Properties for Simulations of Elemental Bismuth Clusters,* J. Kritzer,* R.Q. Topper, New York Chemistry Students' Association of the NY Section of the ACS, Fordham University **(2000). Contributed lecture.**
30. *Benchmarking Potential Energy Models Against Bulk Properties for Simulations of Elemental Bismuth Clusters,* J. Kritzer,* J. de la Parra Jr.*, A. Deaconescu*, D.Coluccio*, S. Mikhail*, K. Demuren*, L. Grinberg*, G. Yu*, R.Q. Topper, Sixth Electronic Computational Chemistry Conference **(1999). Contributed presentation.** (PR)
31. *A Computational Quantum–Chemical Investigation of 2-Acetylaminofluorene,* R. Hannan*, H.-L. Chan*, T. Kiang*, R.Q. Topper, S. Broyde, New York Chemistry Students' Association of the NY Section of the ACS, New York University **(1999). Contributed lecture.**
32. *Adaptive Path-Integral Monte Carlo Methods for Accurate Determination of Molecular Thermodynamic Properties*, R.Q. Topper, 75th meeting of the Florida Section of the ACS, symposium in honor of Prof. DeLos F. DeTar (**1999**). **Invited lecture.** (PR)
33. *Quantum Thermodynamics of Really Hot Molecules*, R.Q. Topper, Fordham University, Department of Chemistry (**1999**). **Invited lecture.**
34. *Making Millions and Making a Difference: What We Can Learn from Peter Cooper*, R.Q. Topper, Henry Whitney Bellows Lecture, Historical Society of the All Souls Unitarian Church (**1999**). **Invited lecture.**
35. *The Trials, Tribulations and Blessings of Undergraduate Research at Predominantly Undergraduate Institutions*, R.Q. Topper, Mesa State College, Faculty Committee on Excellence in Education, Grand Junction, CO (**1999**). **Invited lecture.**
36. *Quantum-Mechanical Investigation of 2-Acetylaminofluorene and Its Adducts,* R.Q. Topper, H.-L. Chan*, T. Kiang*, S. Broyde, 216th national meeting of the ACS, Boston, MA **(1998). Contributed poster.** (PR)
37. *Searching for Signatures of Order-Disorder Phase Transitions in Ammonium Chloride Cation Clusters With Monte Carlo Methods,* D. Bergin*, P. Sweeney*, R.Q. Topper, 216th national meeting of the ACS, Boston, MA **(1998). Contributed poster.** (PR)
38. *Monte Carlo Simulations of Order-Disorder Phase Transitions of Ammonium Chloride Clusters*, R.Q. Topper, Florida State University, Department of Chemistry (**1998**). **Invited lecture.**
39. *Monte Carlo Simulations of Order-Disorder Phase Transitions of Ammonium Chloride Cation Clusters,* D. Bergin*, P. Sweeney*, R.Q. Topper, New York Chemistry Students' Association of the NY Section of the ACS, New York University **(1998). Contributed lecture.**
40. *Effective Uses of Molecular Visualization Tools in Freshman and Physical Chemistry*, R.Q. Topper, Conference on Information Technology, Visualization, and Multimedia in Teaching and Learning, The Information Technologies Cluster, Columbia University, New York, NY (**1997**). **Invited lecture.** (PR)
41. *Computational Molecular Modeling and Theoretical Chemistry in the Undergraduate Chemical Engineering Curriculum*, R.Q. Topper, 213th national meeting of the ACS, San Francisco, CA (**1997**). **Invited lecture.** (PR)
42. *Genetic Algorithm Optimization of Cluster Geometries,* J. Barmash*, E. Agichtein,* R.Q. Topper, New York Chemistry Students' Association of the NY Section of the ACS, New York University **(1998). Contributed lecture.**

43. *Brownian Simplex-Simulated Annealing Studies of Atomic and Molecular Clusters,* F. Torres*, E. Agichtein*, L. Grinberg*, G. Yu,* R.Q. Topper, Third Annual Electronic Computational Chemistry Conference **(1996). Contributed presentation.** (PR)
44. *Cancer, Clusters and Acid Rain: Adventures in Molecular Modeling*, R.Q. Topper, Yale University, Department of Chemistry (**1996**). **Invited lecture.**
45. *Monte Carlo Computations of the Order-Disorder Phase Transition in Solid Ammonium Chloride,* R.Q. Topper, D.L. Freeman, 208th national meeting of the ACS, Washington, DC **(1994). Contributed lecture.** (PR)
46. *Monte Carlo Studies of the Orientational Order-Disorder Transition in Solid Ammonium Chloride*, R.Q. Topper, New York University, Chemical physics colloquium (**1994**). **Invited lecture.**
47. *Quantum Free Energies of Polyatomic Molecules*, R.Q. Topper, University of Rhode Island, Department of Chemistry (January 1993). **Invited lecture.**
48. *Fourier Path-Integral Monte Carlo Computation of Molecular Partition Functions*, R.Q. Topper, D.G. Truhlar, Workshop on Grand Challenges in High Performance Computing and Structural Biology, Tallahassee, FL **(1992). Contributed poster.**
49. *Order, Chaos and Reactive Islands in Molecular Dynamics Simulations*, R.Q. Topper, University of Minnesota, Department of Physics (**1992**). **Invited lecture.**
50. *Quantum Free Energies: Fourier Path-Integral Monte Carlo Computation of Molecular Partition Functions*, R.Q. Topper, University of Minnesota, Department of Chemistry (**1992**). **Invited lecture.**
51. *Fourier Path-Integral Monte Carlo Computation of Molecular Partition Functions*, R.Q. Topper, D.G. Truhlar, Seventh International Conference on Recent Progress in Many-Body Theories, Minneapolis, MN **(1991). Contributed poster.** (PR)
52. *The Reactive Islands Theory of Isomerization Dynamics, Reaction Rates and Population Decays*, R.Q. Topper, Columbia University, Department of Chemistry (**1990**). **Invited lecture.**
53. *Cylindrical Manifolds as Essential Mediators of Microscopic Chemical Reaction Dynamics and Kinetics*, R.Q. Topper, M.A. Mehta, N. De Leon, 201st national meeting of the ACS, Boston, MA **(1990). Contributed poster.** (PR)
54. *Cylindrical Manifolds as Essential Mediators of Microscopic Chemical Reaction Dynamics*, R.Q. Topper, C.C. Marston, M.A. Mehta, N. De Leon, 199th national meeting of the ACS, Miami Beach, FL **(1989). Contributed poster.** (PR)

ORGANIZATION OF CONFERENCES AND SYMPOSIA

1. Invited member of the Scientific Organizing Committee, 14th International Electronic Conference on Synthetic Organic Chemistry (**November 2010**).
2. Principal Organizer, 7th - 11th Electronic Computational Chemistry Conference **(2001–2007).** International "virtual" online conference with hundreds of participants.
3. Invited member of the Scientific Organizing Committee, Fourth Annual Electronic Computational Chemistry Conference (**November 1997**).
4. Invited session chair, *Computational Chemistry in Graduate and Undergraduate Education,* 213th national meeting of the American Chemical Society, San Francisco, CA (**March 1997**).
5. Invited session organizer and online session chair, *"Stochastic Methods for Conformational Sampling,"* First Electronic Molecular Modelling and Graphics Society Conference. This was the first international online chemistry Conference, including real time Q&A sessions with the presenters (**October 1996**).

EXTERNAL FUNDING SUPPORT

1. **Gridchem,** an NSF-supported consortium of national supercomputing institutes. Initial 10,000 SU hour allocation in support of research; renewed annually (**2013-present**). https://www.gridchem.org/ .
2. **AWS in Education Grant**, Amazon Web Services, PI. Computational resource grant in support of neurotransmitter research. Total $1000 (**2013–2015**). https://aws.amazon.com/education/.
3. Three **U.S. Army** / **Academy of Applied Science REAP** // **American Chemical Society SEED grants**. Co-PI: C. Supplee. Total $14,550 (**2006–2007**).
4. Two **U.S. Army** / **Academy of Applied Science REAP** // **Merck SURF grants**. PI. Total $19,700 (**2004–2005**).
5. **Petroleum Research Fund**, Type A supplementary grant for nanocluster research with Mark Johnson, Yale University. Total $6,000 (**2001**).
6. **Petroleum Research Fund**, Type B research grant for nanocluster research. PI. $40,000 (**1998–2001**).

PEER REVIEW ACTIVITY

1. Peer review of research grant proposals for federal agencies, private trusts, nonprofit organizations and universities (most recently, *ACS Petroleum Research Foundation*).
2. Peer review of articles for scientific journals (most recently, *Journal of Chemical Education*)**.**
3. Review of textbook drafts for publishing firms (most recently, *University Science Press*).
4. Review of tenure and promotion packages for faculty at other colleges and universities.

MENTORSHIP

Undergraduate / High School Student Research / Project Advisement:

- **62 undergraduate students** and **51 high school students** have been formally advised in research projects.
- **79%** of the undergraduate students have gone on to graduate studies in chemistry, computer science, engineering, physics, business, medicine, dentistry and law.
- **38** students have published their undergraduate research work in a peer-reviewed journal article and/or presented it at a national or regional scientific conference.
- **Six** former undergraduate research advisees have taken tenure-track STEM faculty positions at MIT, Boston U, Brown, Cooper Union, Georgia Tech, U of Philadelphia.

Graduate Student Advisement:

- Principal thesis advisor to 6 master's students in chemical engineering.
- Outside reader to 2 Ph.D. dissertations / defenses in New York Univ. Biology and Chemistry departments.

Courses Taught At Cooper Union:

- Ch 110, General Chemistry; Ch 111, General Chemistry Lab; Ch 160, Physical Principles of Chemistry
- Ch 261/361, Physical Chemistry I; Ch 262/362, Physical Chemistry II; Ch 370, Inorganic Chemistry
- Ch 391-395 Research Problem I-V; Ch 363/463, Advanced Physical Chemistry; ChE 499 Thesis/Project (Graduate)
- ME 163 Mechanical Engineering Projects; ME 164 Capstone Senior Mechanical Engineering Design

Courses Taught At Monmouth University:

- CE 111, General Chemistry I; CE 111L, General Chemistry I Lab
- CE 112, General Chemistry II; CE 112L, General Chemistry II Lab
- CE 350, Research In Chemistry; CE 401, Advanced Inorganic Chemistry; CE 401L, Advanced Inorganic Chemistry Lab
- CE 475, Computational Chemistry and Molecular Modeling; CE 499, Independent Research In Chemistry
- HO 498, Honors Thesis Proposal; HO 499, Senior Honors Thesis

Courses Taught Elsewhere:

- General Chemistry (I,II); Physical Chemistry (I,II); General Chemistry Laboratory (I,II); and Physical Chemistry Laboratory (I,II) [all as teaching assistant], Yale University (1986-1990).
- Fundamentals of Mathematics, [as teaching assistant], Florida State University and Tallahassee Community College (1984-1986).
- Elements of Photography, Duncan U. Fletcher Community School, Jacksonville Beach, FL (1978).

SERVICE TO THE COOPER UNION

1. Member, Middle States Working Group on Leadership **(2016-present)**.
2. Chair, Institutional Review Board (**2011–present**). Advise faculty, staff and administrators on human subject research issues. Developed new administrative processes, innovative protocols, and best practices for review of human subject research projects. Established a completely online submission and review process.
3. Coordinator, General Chemistry Laboratory **(2001-2003; 2010–present).** Continuously edit and improve the laboratory manual and experiments; recommend equipment purchases; assist adjunct and new FT faculty; coordinate with departmental technicians.
4. Parliamentarian, Faculty of the School of Engineering (**2012–2016**).
5. Member, Promotion and Tenure Committee, School of Engineering (**2010–2014**).
6. Campus Safety Coordinator (**2001–2003**); Engineering School Faculty Safety Coordinator (**1998–2001**). Advised faculty, staff and administrators on all laboratory and studio safety and hazardous waste issues and conducted WRTK and RCRA workshops for students and staff. Maintained NYFD certification for charge of a chemical laboratory.
7. Secretary of the Faculty of the School of Engineering (**1995–2003**). Elected by the Engineering Faculty.
8. Facilitator, Cooper Union/Outward Bound® Engineering and Experiential Learning Project (**1996–2001**). Worked with faculty, students, staff and Outward Bound® staff to provide experiential education experiences to students with a focus on gender, diversity and leadership issues in the engineering professions.
9. Secretary, Committee for Strategic Planning Recommendations (**2001–2003**).
10. Chair, Engineering Faculty Computer Committee (**1999–2003**); regular member (**1994–1999**).
11. Acting Chair, Department of Chemistry (**Summer 1995**).

SERVICE TO MONMOUTH UNIVERSITY

1. Department Chair (**2003–2009**). Supervised a department of 25 faculty and 3 staff; managed annual budget of approximately $1.2M. Evaluated all faculty for promotion/tenure/continuance; steered outcome assessment and six successful ACS program certification reviews; directed all technology acquisitions; coordinated and managed all departmental computer software and hardware acquisitions and maintenance; managed growth of department; steered recruiting efforts; led development of a new degree program in Chemical Physics and a new Minor in Physics; annual reviews of staff; many other duties. The number of departmental majors more than tripled in the period 2003-2011.
2. Chair, Undergraduate Studies Committee (**2008–2009**); regular member (**2003–2009**). All undergraduate courses and curricula university-wide received final review in this committee, which consisted of all of the department chairs and academic deans throughout the University.
3. Coordinator, Medical Technology and Clinical Laboratory Science degree programs (**2005–2009**). Worked closely with faculty at Monmouth Medical Center, UMDNJ and Jersey Shore Medical Center; served on UMDNJ's Clinical Laboratory Science Advisory Committee; steered contractual review and compliance; coordinated information flow between institutions; advised all students during their clinical internships.
4. Served as Acting Dean of the School of Science, Technology and Engineering as needed (**2007–2009**).
5. Member, Joint Biology / Chemistry Advisory Committee (**2008–2009**).
6. Member, University Council of Chairs (**2003–2009**).
7. Member, STE Chairs Committee (**2003–2009**).
8. Coordinator, General Chemistry lecture and laboratory courses (**2003–2009**).
9. Editor and contributor, General Chemistry I and II departmental laboratory manuals (**2005–2009**).
10. Coordination of departmental honors courses; liason to the Honors School; developed first Honors sections of general chemistry lecture and laboratory courses. (**2006–2009**).
11. Director, Monmouth University REAP-SEED Summer Internship in Chemistry Program (**2003–2009**).
12. Member, STE Safety Committee (**2006–2009**).
13. Departmental representative, MU Global Understanding Project (**2005–2008**).
14. Co-Chair, General Education Revision Taskforce (**2005–2006**); member (**2005-2007**).
15. Chair, General Education Oversight Committee (**2005–2006**); member (**2003–2007**).
16. Co-Chair, First Year Experience Taskforce (**2004**).
17. Member, Information Technology Program Director search committee (**2004**).
18. Member, Subcommittee on Faculty, Middle States Accreditation Review Taskforce (**2003–2004**)**.**
19. Member, Monmouth University Ten-Year Strategic Planning Team (**2003–2004**).