Robert Q. Topper

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RESEARCH: ***High-performance computational modeling of complex systems at the molecular level.***

- Physicochemical properties of atmospheric acid-base aerosols formed via homogenous and heterogenous nucleation in polluted urban environments.
- Free software for highly ergodic algorithms for structure prediction.
- Thermodynamic, spectral, and structural properties of compounds and nanoclusters via density functional theory and coupled-cluster methods.
- Machine learning methods for prediction and analysis of free energy surfaces of biomolecules and materials.
- Stochastic process algorithms for quantum and classical statistics and mega-dimensional integration problems via quantum and classical Monte Carlo methods.
- Nonlinear dynamics, chaos, and reaction rates.
- DNA damage caused by environmental mutagens and carcinogens found in tobacco smoke and grilled meats.

PROFESSIONAL EMPLOYMENT SUMMARY

2009 – Present	**Professor,** School of Engineering, The Cooper Union. Tenured.
2017	**Visiting Research Professor**, Department of Chemistry, New York University.
2010 – 2019	**Chair, Institutional Review Board**, The Cooper Union. Appointed position.
2003 – 2009	**Chair and Associate Professo**r, Department of Chemistry, Medical Technology, and Physics, Monmouth University (NJ). Tenured.
1999 – 2003	**Associate Professor**, School of Engineering, The Cooper Union. Tenured.
1998 – 2003	**Campus Safety Coordinator**, The Cooper Union. RCRA/OSHA/WRTK training & compliance. Appointed position.
1993 – 1999	**Assistant Professor**, School of Engineering, The 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.
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**).	Advisor: Nelson De Leon.
M.S., M.Phil., Physical Chemistry, Yale University (**1989**).	
B.S., Physics and Chemistry, Florida State University (**1986**).	Advisors: DeLos F. DeTar, Robley Light, Jack Saltiel.

HONORS, FELLOWSHIPS AND AWARDS

Cooper Union Engineering Student Council Student's List for Exemplary Teaching (**2010** and **2012**); Phi Lambda Upsilon (**2008**); Order of the Engineer, for outstanding contributions to engineering education (**2001**); Minnesota Supercomputing Institute Research Fellow (**1990-1992**); William Kent Research Fellow, Yale University (**1989-1990**); Robert B. Flint Graduate Fellow, Yale (**1986–1990**); Florida State University College of Arts and Sciences Leadership Award (**1986**); FSU American Institute of Chemists Award (**1986**); Charles A. Brautlecht and Louise I. Brautlecht Scholarship in Chemistry Research (**1985-1986**); Sigma Pi Sigma (**1985**); National Merit Scholar (**1981-1985**).

MENTORSHIP

- **69 undergraduate students** and **52 high school students** have been formally advised in research to date.
- Of these, **48 have earned graduate degrees and 11 attained full-time STEM faculty positions.**
- Principal research advisor or co-advisor to **10 master's students** at Cooper Union.
- Dissertation reader and informal advisor and mentor to Ph.D. students at New York University.

COLLABORATIONS (* = research was grant supported and/or resulted in publications)

Greg A. Moehring	Chemistry and Physics	Monmouth University	2022-present
Datta Naik	Chemistry and Physics	Monmouth University	2022-present
Mark Tuckerman*	Chemistry and Mathematics	New York University	2017-present
Donald G. Truhlar*	Chemistry	University of Minnesota	1994-present
David L. Freeman*	Chemistry	University of Rhode Island	1993-2003
Mark A. Johnson*	Chemistry	Yale University	2000-2002

ARTICLES AND BOOK CHAPTERS (*=undergraduate coauthor, **=high school student coauthor)

- A. Hassan*, S.L. Topper, R.Q. Topper, *Computational analysis of mass spectra and growth patterns of ammonium nitrate nanoparticles*, ***Journal of Physical Chemistry A*** **(in preparation, 2023).**
- R.Q. Topper, S.L. Topper, S. Lee*, *TransRot: A portable software package for simulated annealing Monte Carlo geometry optimization of atomic and molecular clusters*, in ***Physical Chemistry Research at Undergraduate Institutions: Innovative and Impactful Approaches Vol.1****,* T. Hopkins and C.A. Parish, Eds., Chapter 2, pp, 19-38, ACS Symposium Series Vol. 1428 (**2022**)**.** eISBN: 9780841297425
- A.J.V. Lomboy*, R.Q. Topper, *Nonuniform proton transfer and strong hydrogen bonding within cation, anion, and neutral clusters of ammonia and hydrogen fluoride*, ***Journal of Physical Chemistry A***, 125(12), pp. 2546-2557 (**2021**). DOI: 10.1021/acs.jpca.1c00732.
- J.R. Cendagorta, J. Tolpin*, E. Schneider, R.Q. Topper, M.E. Tuckerman, *Comparison of the performance of machine learning models in representing high-dimensional free energy surfaces and generating observables*, ***Journal of Physical Chemistry B,*** 124(18)**,** pp.3647-3660 (**2020**). DOI: 10.1021/acs.jpcb.0c01218
- 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**). DOI: 10.1103/PhysRevLett.119.150601
- 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**). DOI: 10.1021/acs.jpca.6b06788
- R.Q. Topper, W. V. Feldmann*, I. Markus*, 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)**. DOI: 10.1021/jp2069732
- 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).** DOI: 10.1016/j.theochem.2004.08.005
- S. Ling, R.Q. Topper, *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
- R.Q. Topper, D.L. Freeman, D. Bergin, K. LaMarche*, *Computational techniques and strategies for Monte Carlo thermodynamic calculations with applications to nanoclusters*, in ***Reviews in Computational Chemistry***, Vol. 19, Chapter 1, 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
- 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).** DOI: 10.1007/s00214-002-0409-z
- 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)**. See https://web.archive.org/web/20070418052350/http://www.ijc.com/articles
- R.Q. Topper, *Adaptive path-integral Monte Carlo methods for accurate computation of molecular thermodynamic properties*, in ***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)**. ISBN-13: 978-0471196303

- 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)**. DOI: hS0166-1280(97)00195-4
- R.Q. Topper, *Visualizing molecular phase space: Non–statistical effects in reaction dynamics,* in ***Reviews in Computational Chemistry***, Vol. 10, Chapter 3, pp. 101-176, K.B. Lipkowitz and D.B. Boyd, Eds., VCH Publishers, New York **(1997)**. ISBN:9780471186489
- A. Matro, D.L. Freeman, R.Q. Topper, *Computational study of the structures and thermodynamic properties of ammonium chloride clusters using a parallel jump-walking approach,* ***Journal of Chemical Physics*** 104, 8690 **(1996)**. DOI: 10.1063/1.471558
- 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 published elsewhere but was widely disseminated and has been cited in the primary literature. https://arxiv.org/abs/chem-ph/9403002
- 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)**. DOI: 10.1063/1.464953
- 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)**. DOI: 10.1063/1.462949
- 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)**. DOI: 10.1063/1.462948
- 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)**. DOI: 10.1063/1.460065
- 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)**. DOI: 10.1063/1.460116

PUBLISHED SOFTWARE, EDUCATIONAL MATERIALS AND BOOK REVIEWS (*=undergraduate coauthor)

- R.Q. Topper, I. Markus, *Annie 4.7.1*, https://engfac.cooper.edu/topper/Publications (**2022**).
- S.L. Topper*, R.Q. Topper, *TransRot,* https://github.com/steventopper/Transrot (**2021**).
- 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. Workshop product; peer reviewed.
- 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. Workshop product; peer reviewed.
- R.Q. Topper, *Trends in Measured Redox Potentials and Computed Molecular Orbital Energies of Derivatized Buckminsterfullerene****, http://www.ionicviper.org*** **(2013).** Contributed learning object, peer reviewed.
- *"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)**. Invited book review; edited.
- *"Reviews in Computational Chemistry, Vol. 13,"* ***Journal of the American Chemical Society,*** **122**(19), 4845 **(2000)**. Invited book review; edited.
- *"Mathematica Computer Programs for Physical Chemistry,"* ***Theoretical Chemistry Accounts,*** **101**, 439 **(1999)**. Invited book review; edited.
- *"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).** Invited book review; edited.

ORGANIZATION OF CONFERENCES AND SYMPOSIA

- Organising team member, **Virtual Winter School on Computational Chemistry** (**2022-present**). See https://winterschool.cc/team .

- Invited member of the Scientific Organizing Committee, **14th International Electronic Conference on Synthetic Organic Chemistry** (**November 2010**).
- Principal Organizer, **7th - 11th Electronic Computational Chemistry Conference (2001–2007).**
- Invited member of the Scientific Organizing Committee, **Fourth Annual Electronic Computational Chemistry Conference** (**November 1997**).
- Invited session chair, *Computational Chemistry in Graduate and Undergraduate Education,* **213th national meeting of the ACS**, San Francisco, CA (**March 1997**).
- Invited session organizer and online session chair, *"Stochastic Methods for Conformational Sampling,"* **First Electronic Molecular Modelling and Graphics Society Conference**. (**October 1996**).

EDITED CONFERENCE PROCEEDINGS (**=high school student coauthor)

- *Abstracts of the **11th Electronic Computational Chemistry Conference**,* R.Q. Topper, and O. Dmitrenko, Eds., *http://stores.lulu.com/eccc* (**2008**). (PR)
- 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)
- 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)
- *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)
- 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)

INVITED TALKS (PR = abstract was peer reviewed).

- *Stochastic simulation, quantum mechanics, and machine learning approaches to intra-cluster proton transfer and conformational diversity*. **Department of Chemistry, New Jersey Institute of Technology, Newark NJ (2019).**
- *Stochastic searching and machine learning methods for acceleration and analysis of atomistic simulations*. **Department of Chemistry, The College of New Jersey, Ewing NJ (2018).**
- *Molecular modeling of nanoparticles and polypeptides*. **Department of Chemistry, University of Rhode Island, Kingston RI (2017)**.
- *Computational and theoretical physical chemistry: Applications to ammonium halide nanoclusters*. **High Technology High School, Lincroft, NJ (2017)**.
- *Computational studies of structural diversity in nanoparticles of ammonium halides*. **Department of Chemistry, Queensborough Community College**, **Bayside, NY (2014**).
- *Strategies for Engaging, Leading, and Supporting Undergraduate and High School Students in Computational and Theoretical Chemistry Research Projects*. **230th national ACS meeting, Washington, D.C. (2005).** PR
- *Modeling DNA damage: Computational cascade analyses of N-Acetyl-2-Aminofluorene (AAF) adducts to guanine and deoxyguanosine.* **Department of Chemistry and Minnesota Supercomputer Institute, Symposium on Computational Chemical Dynamics, University of Minnesota**, **Minneapolis MN (2004).** PR
- *Monte Carlo quantum thermodynamics of really hot molecules*. **Department of Chemistry, University of Memphis**, **Memphis TN (2001).**
- *Adaptive path-integral Monte Carlo methods for accurate determination of molecular thermodynamic properties*. **75th meeting of the Florida Section of the ACS, Florida Award Symposium, Orlando FL** (**1999**). PR
- *Quantum thermodynamics of really hot molecules*. **Department of Chemistry, Fordham University, New York NY** (**1999**).
- *Making millions and making a difference: What we can learn from Peter Cooper*. **Henry Whitney Bellows Lecture, Historical Society of the All Souls Unitarian Church, New York NY** (**1999**).

- *The trials, tribulations and blessings of undergraduate research at predominantly undergraduate institutions*. **Faculty Committee on Excellence in Education, Mesa State College, Grand Junction, CO (1999)**.
- *Monte Carlo simulations of order-disorder phase transitions in ammonium chloride clusters*. **Department of Chemistry, Florida State University, Tallahassee FL** (**1998**).
- *Effective uses of molecular visualization tools in freshman and physical chemistry*. **Conference on Information Technology, Visualization, and Multimedia in Teaching and Learning, The Information Technologies Cluster, Columbia University, New York, NY (1997).** PR
- *Cancer, clusters and acid rain: Adventures in molecular modeling*. **Department of Chemistry, Yale University, New Haven CT** (**1996**).
- *Monte Carlo studies of the orientational order-disorder transition in solid ammonium chloride*. **Department of Chemistry, New York University, New York NY (1994**).
- *Quantum free energies of polyatomic molecules*. **Department of Chemistry, University of Rhode Island**, **Kingston RI (1993).**
- *Order, chaos and reactive islands in molecular dynamics simulations*. **Department of Physics, University of Minnesota, Minneapolis MN (1992).**
- *Quantum free energies: Fourier path-integral Monte Carlo computation of molecular partition functions*. **Department of Chemistry, University of Minnesota, Minneapolis MN (1992).**
- *The Reactive Islands theory of isomerization dynamics, reaction rates and population decays*. **Department of Chemistry, Columbia University**, **New York NY** (**1990**).

CONTRIBUTED TALKS (presenters' names underlined; *=undergraduate coauthor, **=high school student coauthor; PR=peer reviewed).

- *Computational analysis of mass spectra and growth patterns of ammonium nitrate nanoparticles*, A. Hassan* and R.Q. Topper, 70th Annual Undergraduate Research Symposium of the New York section of the American Chemical Society, LaGuardia Community College, New York NY **(submitted, 2023).** PR
- *Software for ergodic simulated annealing Monte Carlo calculations of atomic and molecular clusters and nanoparticles*. R.Q. Topper, **2022 Middle Atlantic Regional Meeting (MARM) of the ACS**, The College of New Jersey, Ewing NJ **(2022).** PR
- *Mag-walking simulated annealing Monte Carlo study of nano-solvated ammonium chloride*. S. Lee,* S.L. Topper, R.Q. Topper, **69th Annual Undergraduate Research Symposium of the New York section of the American Chemical Society,** Medgar Evers College, New York NY **(2022).** PR
- *Sometimes a salty nanoparticle is only "sort of salty", and sometimes engineers are interested in theoretical chemistry*. R.Q. Topper, **Fall 2021 Meeting of the American Chemical Society, Atlanta GA (2021).** PR
- *Modeling atmospheric nanoparticles: Characterizing proton transfer in ammonium fluoride nanoclusters*. A.J. Lomboy* and R.Q. Topper**, 66th Annual Undergraduate Research Symposium of the New York section of the American Chemical Society,** Queensborough NY **(2018).** PR
- *Unusual hydrogen bond diversity in ammonium halide nanoclusters*. R.Q. Topper, J.J. Biswakarma,* **57h Sanibel Symposium**, **University of Florida Quantum Theory Project, St. Simons Island GA (2017)**. PR
- *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 ACS**, College of St. Vincent, Riverdale NY **(2016).** PR
- *Relative proton acidities within a bicyclic thioacetal*. B. Lee*, R.Q. Topper**, 63rd Annual Undergraduate Research Symposium of the New York section of the American Chemical Society**, Queensborough Community College, Queensborough NY **(2015)**. PR
- *Solvent effects on neurotransmitter conformations*. S. Sharif*, R.Q. Topper, **62nd Annual Undergraduate Research Symposium of the New York section of the American Chemical Society,** Queensborough Community College, **Queensborough NY** (**2014**). PR
- *Computational modeling of covalent deoxyguanosine adducts.* R.Q. Topper**,** T.A. Isgro, N. Mathew**, **226th national meeting of the ACS**, **New York, NY (2003).** Abstract published in ***Chemical Research in Toxicology*** **17(12)**; 1757-1783 **(2004)**. Dedon, P. C.; Penning, T. M., eds. PR
- *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). Online.** PR

- *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).** PR
- *Benchmarking potential energy models against bulk properties for simulations of elemental bismuth clusters.* J. Kritzer,* R.Q. Topper, **48th Annual Undergraduate Research Symposium of the New York section of the American Chemical Society**, **Fordham University, New York NY (2000).** PR
- *A computational quantum–chemical investigation of 2-acetylaminofluorene.* R. Hannan*, H.-L. Chan*, T. Kiang*, R.Q. Topper, S. Broyde, **47th Annual Undergraduate Research Symposium of the New York section of the American Chemical Society, New York University, New York NY (1999).** PR
- *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). Online.** PR
- *Monte Carlo simulations of order-disorder phase transitions of ammonium chloride cation clusters.* D. Bergin*, P. Sweeney*, R.Q. Topper, **46th Annual Undergraduate Research Symposium of the New York section of the American Chemical Society**, **New York University (1998).** PR
- *Genetic algorithm optimization of cluster geometries.* J. Barmash*, E. Agichtein,* R.Q. Topper, **46th Annual Undergraduate Research Symposium of the New York section of the American Chemical Society**, New York University **(1998).** PR
- *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**). PR
- *Brownian simplex-simulated annealing studies of atomic and molecular clusters.* F. Torres*, E. Agichtein*, L. Grinberg*, G. Yu,* R.Q. Topper, **Third Electronic Computational Chemistry Conference (1996). Online.** PR
- *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).** PR
- *Trans-esterification and formal steric enthalpy*. R.Q. Topper and D.F. DeTar, **18th Annual ACS Southeast Undergraduate Research Conference, University of South Alabama, Mobile, AL (1986)**. PR

POSTER PRESENTATIONS (presenters' names underlined; PR = abstract or presentation was peer reviewed; * = undergraduate coauthor, **=high school student coauthor)

- *TransRot: a portable and easy-to-use open source software package for simulated annealing Monte Carlo geometry optimization of nanoparticles*. S. Lee,* S.L. Topper, R.Q. Topper, **10th Triennial Conference on Molecular Quantum Mechanics, Blacksburgh, VA (2022)**. PR
- *TransRot: Machine-portable software for sawtooth simulated annealing-magwalking Monte Carlo optimizations of clusters*. R.Q. Topper, S.L. Topper, **2022 Virtual Winter School on Computational Chemistry**, held online at https://winterschool.cc/program-2022 (**2022**).
- *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 ACS**, San Francisco, CA (**2014**). PR
- *A computational study of the structure of tetrakisdiethylamidozirconium*. A. Grofe*, N. Rao, R.Q. Topper, C.A. Smith*, **Sigma Xi Research Symposium at Saint Joseph University**, Philadelphia, PA (**2012**). **Contributed student poster.** PR
- *Structures, spectra, reaction energies and oxidation trends of NH_4Cl nanocrystallites*. R.Q. Topper, W.V. Feldmann,* I. Markus,* **240th national meeting of the ACS**, Boston, MA (**2010**). PR
- *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**). PR
- *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**). PR
- *Structural properties of ammonium chloride clusters.* C. Russamano,* R.Q. Topper**, Second Annual SURF Symposium, Merck Inc,.** Rahway, NJ (**2005**).
- *Computational modeling of deoxyguanosine adducts*. N. Jain,* R.Q. Topper**, First Annual SURF Symposium, Merck Inc.,** Rahway, NJ **(2004)**.

- *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)**. PR
- *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,** Tannesrville, PA **(2002).** PR
- *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 ACS**, Washington, DC. **(2000).** PR
- *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).** PR
- *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).** PR
- *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**, **Florida State University, Tallahassee FL (1992).** PR
- *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).** PR
- *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). Including computer-generated animations, this was the first multimedia poster presentation ever given at a meeting of the ACS.** PR
- *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).** PR

EXTERNAL FUNDING AND PENDING PROPOSALS

- **RUI: Dynamic processes and bond activation within rhenium polyhydride complexes**, with Greg Moehring and Datta Naik (collaboration with Monmouth University) **(NSF, in prepraration).** Co-PI.
- **Gridchem,** an NSF-supported consortium of national supercomputing institutes (**2013-2018**). https://www.gridchem.org/ . Cloud-based computational resource grant.
- **AWS in Education Grant**, Amazon. PI; Cloud-based computational resource grant in support of neurotransmitter research. Total $1000 (**2013–2015**). https://aws.amazon.com/education/.
- **IONIC-VIPER**, an NSF-supported consortium of chemistry educators. Competitive grant awarded to participate in the **2013 VIPER Workshop for Alternative Energy Needs** at Pennsylvania State University (**2013**).
- Three **U.S. Army** / **Academy of Applied Science REAP** // **American Chemical Society SEED grants**. Co-PI: C. Supplee. Total $14,550 (**2006–2007**).
- Two **U.S. Army** / **Academy of Applied Science REAP** // **Merck SURF grants**. PI. Total $19,700 (**2004–2005**).
- **Petroleum Research Fund of the American Chemical Society**, Type A supplementary grant for nanocluster research. Co-PI: Mark Johnson, Yale University. Total $6,000 (**2001**).
- **Petroleum Research Fund**, Type B research grant for nanocluster research. PI. $40,000 (**1998–2001**).

PROFESSIONAL ACTIVITY, OUTREACH, and VOLUNTEER WORK

- Peer review of research grant proposals for federal agencies, private trusts, nonprofit organizations and universities (most recently, ***ACS Petroleum Research Foundation*** and ***National Science Foundation***).
- Peer review of articles for scientific journals (most recently, ***Chaos: An Interdisciplinary Journal*****).**
- Review of textbook drafts for publishing firms (most recently, ***Taylor / CRC Press*** and ***ACS Monograph Series***).
- Departmental and program reviews for other colleges and universities (***Iona College***)
- Review of tenure and promotion packages for faculty at other colleges and universities (***Thomas Jefferson University***).
- Consultant for development of materials and modules for teaching physical chemistry (***Monmouth University)*****.**
- Executive Board member, New Jersey State Youth Orchestra **(2017-2020).**
- Volunteer scientist, NEWTON Ask A Scientist, Argonne National Laboratories **(1993-2015)**.
- Research leader, Cooper Union High School Summer Research Program **(1993-2003)**.
- Judge, New York Science and Technology Expo **(1998 and 2000)**.

SERVICE TO COOPER UNION (1993-2003; 2009-present)

- Secretary, School of Engineering **(1995-2003, 2021-present).** Elected.
- Parliamentarian, School of Engineering **(2012-present).** Apoointed and re-appointed by five deans.
- Engineering Curriculum Committee **(2022-present)**.
- Course Coordinator, General Chemistry Laboratory **(2001-2003; 2010-present).**
- Engineering Academic Standards Committee **(2018-2022)**.
- Engineering Promotion and Tenure Committee **(2010-2013)**.
- Chair, Institutional Review Board **(2010-2019).** Appointed by VPFA & Treasurer Theresa Westcott.
- Campuswide Safety Coordinator **(1998-2003).** Appointed by VPBA Robert Hawks.
- Facilitator, Cooper Union/Outward Bound® Engineering and Experiential Learning Project (**1996-2001**).
- Secretary of the Committee for Strategic Planning Recommendations (**2001–2003**).
- Chair, Engineering Faculty Computer Committee (**1999–2003**); member (**1994-1999**).
- Member, Faculty External Awards Nominating Committee (**1995–2001**).
- Acting Chair, Department of Chemistry (**Summer 1995**).

SERVICE TO MONMOUTH UNIVERSITY (2003-2009)

- Department Chair (**2003-2009**). Supervised a department of 28 faculty and staff; annual budget $1.2M.
- Chair (elected), Undergraduate Studies Committee (**2008-2009**); regular member (**2003-2009**).
- 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 as Acting Dean of the School of Science, Technology and Engineering upon request of the Dean (**2007-2009**).
- Member, Joint Biology / Chemistry Advisory Committee (**2008-2009**).
- Member, University Council of Chairs (**2003-2009**).
- Member, STE Chairs Committee (**2003-2009**).
- Coordinator, General Chemistry lecture and laboratory courses (**2003-2009**).
- Editor and contributor, General Chemistry I and II departmental laboratory manuals (**2005-2009**).
- Coordinator of departmental honors courses, and liason to the Honors School (**2006-2009**).
- Director, Monmouth University REAP-SEED Summer Internship in Chemistry Program (**2003-2009**).
- Member, STE Safety Committee (**2006-2009**).
- Departmental representative, MU Global Understanding Project (**2005-2008**).
- Co-Chair, General Education Revision Taskforce (**2005-2006**); member (**2005-2007**).
- Chair, General Education Oversight Committee (**2005-2006**); member (**2003-2007**).
- Co-Chair, First Year Experience Taskforce (**2004**).
- Member, Information Technology Program Director search committee (**2004**).
- Member, Subcommittee on Faculty, Middle States Accreditation Review Taskforce (**2003-2004**)**.**
- Member, Monmouth University Ten-Year Strategic Planning Writing Team (**2003-2004**).

ORGANIZATIONS

- Alpha Chi Sigma
- American Chemical Society
- Order of the Engineer
- Phi Lambda Upsilon
- Sigma Pi Sigma