

## Bala Ramu Ramachandran

*Associate Vice President for Research and  
Dean of the Graduate School  
Director, Institute for Micromanufacturing  
T. L. James Eminent Scholar Chair Professor  
Louisiana Tech University,  
Ruston, LA 71272 USA*



### **CONTACT INFORMATION:**

P.O. Box 7923

Louisiana Tech University

Ruston, LA 71272

**Phone:** (318) 257-4304

**E-mail:** [ramu@latech.edu](mailto:ramu@latech.edu)

**Web page:** [www2.latech.edu/~ramu](http://www2.latech.edu/~ramu)

### **PERSONAL:**

US Citizen, Married, 3 boys 24, 20, 14

### **EDUCATION:**

B.Sc., Chemistry, University of Calicut, India, June 1980

M.Sc., Chemistry, Indian Institute of Technology, Madras, India, May 1982

Ph.D., Chemistry, Kansas State University, Manhattan, Kansas, December 1987

Post-Doctoral Research Fellow, University of Texas, Austin, Texas, 1987-89

### **HONORS/AWARDS**

Chemistry Department Award for Excellence in Teaching, 1984

Chemistry Department Award for Excellence in Research, 1985

Phi Lambda Upsilon Graduate Research Award, 1986

Louisiana Tech University Foundation Professorship, 2002 (nominated by colleagues)

Marquis Who's Who in Science & Engineering, 2004-present

Academic Keys Who's Who in Higher Education, 2004-present

W.W. Chew Board of Regents Endowed Professorship, 2004-2007

Hazel Stewart Garner Board of Regents Endowed Professorship, 2007-2017

T. L. James Eminent Scholar Chair Board of Regents Endowed Professorship, 2017-present

### **ADMINISTRATIVE EXPERIENCE (Reverse Chronological):**

**June 2019-present: Director, Institute for Micromanufacturing**

#### *Main functions:*

- Coordinate the external funding efforts of the Institute by facilitating and supporting faculty teams.
- Supervise the technical staff of the Institute to ensure that shared major equipment availability is as high as possible (target of 90%).
- Supervise administrative staff of the Institute to ensure that faculty and students are provided adequate administrative support for conducting research (purchasing, travel, etc.).

- Administer the Institute's budgets – operating, cost-recovery center, and gifts.
- Review and approve research proposals and research contracts.
- Lead or coordinate major research instrument proposal initiatives.

**July 2017-present: Associate Vice President for Research and Dean of Graduate School**

***Main functions:***

Research Enterprise:

- Serve as member of Administrative & Planning Council, President's Leadership Team.
- Provide strategic support to existing and emerging centers in subject areas of focus (Energy, Infrastructure, Materials).
- Represent LaTech in ongoing engagement and facilitation of partnerships with the Louisiana EPSCOR Committee and Southeastern Universities Research Association.
- Co-lead the University's Sponsored Programs Council with AVP/Research & Partnerships to develop and support functions and strategies for the research enterprise.
- Hold review and approval authority for proposals in designated subject areas.
- Serve on the Biosafety and Radioisotope Institutional Review Committee. Contribute to quarterly update meeting on overall research compliance issues.
- As needed, provide input and advice to Office of Sponsored Programs on improving efficiencies of research administration and processes.
- Support and advise the CRIO on strategic, operational, and organizational issues for the Research Enterprise.

Graduate School:

- Oversee and coordinate graduate student recruitment efforts to meet the University's targets for growth.
- Oversee administration of graduate application reviews and admissions processes.
- Lead the University Graduate Council; provide leadership to the Associate Deans for Graduate Studies across all colleges.
- Administer the awarding of degrees and monitoring of academic standards in graduate programs.
- Promote and develop new interdisciplinary graduate programs in relevant and sustainable areas; promote opportunities and support infrastructure for offering of online graduate programs with significant growth potential.
- Develop and implement strategies for effectively integrating research and graduate education.
- Serve on the Council of Academic Deans.

**July 2013-June 2017: Executive Associate Dean for Research, College of Engineering & Science**

***Main functions:***

- Coordinate the efforts of the College research centers, and leverage their budgets for maximum benefit to the institution
- Work closely with the VP for Research and Economic Development on strategic initiatives.
- Review and approve research proposals and research contracts.
- Coordinate and facilitate the activities of the College Research and Development (RED) team and subteams.
- Monitor and propose improvements to the research infrastructure; ensure the strategic use of College research support budget.

- Monitor and enforce the safety and compliance policies of the Institutional Review Board (animal and human subjects) and Biosafety and Radioisotope Institutional Review Committee (includes purchase, storage, and use of nanoparticles and nanotubes in research).
- Coordinate activities of research centers and provide leadership for major research proposal initiatives.
- Represent the College on the Research Council.

**July 2008-June 2013: Associate Dean for Research, College of Engineering & Science**

***Main functions:***

- Review and approve research proposals and research contracts.
- Coordinate and facilitate the activities of the College Research and Development (RED) team and subteams.
- Monitor and propose improvements to the research infrastructure; ensure the strategic use of College research support budget.
- Monitor and enforce the safety and compliance policies of the Institutional Review Board (animal and human subjects) and Biosafety and Radioisotope Institutional Review Committee (includes purchase, storage, and use of nanoparticles and nanotubes in research).
- Coordinate activities of research centers and provide leadership for major research proposal initiatives.
- Represent the College on the Research Council.
- Oversee the research infrastructure budget of the College.
- Work closely with the VP for Research and Economic Development on strategic initiatives.

**June 2003-June 2017: Program Chair, Molecular Sciences and Nanotechnology (MSNT)**

***Main functions:***

- Schedule and coordinate graduate courses supporting the MSNT program.
- Review and recommend action on applications for admission to the MSNT program.
- Review and approve plans of study, advisory committees, MS theses in the MSNT program.
- Coordinate and facilitate the meetings of the MSNT Steering Committee.
- Provide leadership for the curricular and research activities of the program.

**February 2009-April 2010: Acting Director, Institute for Micromanufacturing (IfM)**

***Main functions:***

- Act as Dean's representative at the IfM, ensuring smooth and effective flow of information from the Institute to the College Leadership Team and vice versa until a permanent director is hired.
- Manage the budget of the Institute.
- Work with the Associate Director of Operations to maximize the availability of the resources of the Institute as possible for faculty and student research.
- Organize faculty/staff teams and provide leadership and guidance for responding to major funding opportunities that leverage the Institute's strengths in micro- and nanotechnology.
- Organize and facilitate the bi-weekly meetings of the IfM Leadership Team.
- Organize and facilitate the bi-weekly meetings of the IfM faculty, staff, and students.

- Work closely with the VP for Research and Economic Development on strategic initiatives of the Institute.

**July 2004-June 2008: Associate Dean for Research & Graduate Studies, College of Engineering & Science**

***Main functions:***

- Enforce College and University regulations in matters related to graduate admissions and administration of graduate programs.
- Oversee the recruiting and retention efforts of the College pertaining to graduate students.
- Manage the College budget for graduate assistantships; make sure that the funds are distributed in a manner supportive of the strategic goals of the College and University.
- Coordinate and facilitate the functions of the College Graduate Studies (GRAD) team.
- Coordinate the scheduling of interdisciplinary graduate courses.
- Represent the College on the Graduate Council.
- Review and approve research proposals and research contracts.
- Coordinate and facilitate the activities of the College Research and Development (RED) team and subteams.
- Monitor and propose improvements to the research infrastructure; ensure the strategic use of College research support budget.
- Coordinate activities of research centers and provide leadership for major research proposal initiatives.
- Represent the College on the Research Council.
- Oversee the research infrastructure budget of the College.

**February 2002-June 2004: Director of Graduate Studies, College of Engineering & Science**

***Main functions:***

- Enforce College and University regulations in matters related to graduate admissions and administration of graduate programs.
- Oversee the recruiting and retention efforts of the College pertaining to graduate students.
- Manage the College budget for graduate assistantships; make sure that the funds are distributed in a manner supportive of the strategic goals of the College and University.
- Facilitate the functions of the College Key Strategic Direction 2 (Graduate Studies) team.
- Coordinate the scheduling of interdisciplinary graduate courses.
- Represent the College on the Graduate Council.

**July 1998-June 2004: Academic Director for Chemistry & Physics**

(Served in an interim capacity from July 1998 to June 2000)

***Main functions:***

- Provide leadership to the program faculty and attempt to address their concerns in a timely and professional manner.
- Mentor the program faculty and actively encourage their participation in interdisciplinary research teams.
- Work with the Program Chairs of the two programs to ensure that classes are scheduled and staffed adequately.
- Ensure that the workloads of program faculty are distributed in a fair and equitable manner.
- Conduct annual faculty evaluations for faculty in the two programs.
- Make recommendations to the Dean regarding hiring, tenure, promotion, and pay raises for faculty in the two programs.

- As a member of the College Leadership Team, work to ensure the success of the College Strategic Plan.
- As a member of the College Leadership Team, take specific responsibility for progress in one or more Key Strategic Directions of the College Strategic Plan.
- As a member of the College Leadership Team, make recommendations regarding the allocation and participate in the management of the operating budget of the College.

**July 1996–June 1998: Program Chair of Chemistry**

***Main functions:***

- Provide leadership in all matters concerning undergraduate and graduate curricula of the program including curriculum development and reform.
- Schedule classes and make recommendations to the Academic Director regarding the teaching assignments of program faculty.
- Ensure that proper advising is available to all students in the program.
- Provide leadership in the recruiting efforts of the program.
- Prepare reports required by the College or University administration in matters such as “Duplicate Program Review” or “Low-completer Program Review.”
- Ensure that required steps are taken to honor collaborative agreements with other campuses.

**ACADEMIC CAREER (Reverse Chronological):**

**July 2003–present: Professor of Chemistry**

***Main functions:***

- Responsible for teaching undergraduate and graduate physical chemistry classes, laboratories, and independent study classes.
- Responsible for maintaining an acceptable level of scholarly activity such as research, publication, and attempts to secure funding for research.
- Submit proposals to funding agencies to secure external funding for research, equipment, and student support.
- Mentor new tenure-track faculty so as to ensure their success both in the classroom and in research.
- Participate in the activities required to maintain and advance the program such as recruiting students, maintaining and improving the teaching/laboratory facilities, and curriculum development and reform.
- Participate in teams/committees at the program, college or university level as the need arises.
- Provide leadership for the curricular and research activities of the program.

**July 1993–June 2003: Associate Professor of Chemistry**

***Main functions:***

- Responsible for teaching undergraduate and graduate physical chemistry classes, laboratories, and independent study classes.
- Responsible for maintaining an acceptable level of scholarly activity such as research, publication, and attempts to secure funding for research.
- Submit proposals to funding agencies to secure external funding for research, equipment, and student support.
- Mentor new tenure-track faculty so as to ensure their success both in the classroom and in research.

- Participate in the activities required to maintain and advance the program such as recruiting students, maintaining and improving the teaching/laboratory facilities, and curriculum development and reform.
- Participate in teams/committees at the program, college or university level as the need arises.

**September 1989–July 1993: Assistant Professor of Chemistry**

***Main functions:***

- Responsible for teaching undergraduate and graduate physical chemistry classes, laboratories, and independent study classes.
- Responsible for maintaining an acceptable level of scholarly activity such as research, publication, and attempts to secure funding for research.
- Participate in the activities required to maintain and advance the program such as recruiting students, maintaining and improving the teaching/laboratory facilities, and curriculum development and reform.
- Participate in teams/committees at the program, college or university level as the need arises.

**HONORARY SOCIETIES**

Phi Lambda Upsilon (Chemistry Honor Society)

Sigma Xi

**PROFESSIONAL SOCIETIES**

American Physical Society (APS)

American Chemical Society (ACS)

American Society for Engineering Education (ASEE)

**GRANTS:**

- 1990-91: A new variational method for calculating reaction cross-sections, LaSER/NSF grant, \$7,000.00
- 1989-92: Three Faculty Development Grants totalling \$3860.00 and three Summer Research Grants totaling \$2,500.00, from Louisiana Tech University.
- 1991-92: Stipends totaling \$3,500 from the Institute for Theoretical Chemistry, University of Texas at Austin, Texas, for conducting collaborative research with Professor Robert E. Wyatt, Director of the Institute for Theoretical Chemistry.
- 1993-94: *Enhancement of Physical Chemistry Courses*, LEQSF Enhancement Grant, \$35,000.
- 1994-97: *Reaction dynamics of the HClO system*, LEQSF Research Grant, \$62,000.
- 1997-00: *Reaction, isomerization, and photoabsorption dynamics of the HOCl molecular system in the ground singlet state*, National Science Foundation, \$113,200. [CHE-9712764]
- 1999-00 *Acquisition of a Fourier Transform Infrared Spectrometer* (with Gene A. Crowder), BoRSF Enhancement Grant, \$20,400.
- 1999-00 *A joint proposal to enhance the computational content in chemistry courses* (with Richard E. Norman of NLU), BoRSF Enhancement Grant, \$16,893.

- 1999-00 *Spectrophotometry equipment for chemistry laboratories* (with L. Dale Snow, Upali Siriwardane, and Gene A. Crowder), BoRSF Enhancement Grant, \$24,900.
- 2002-03 *Enhancement of physical chemistry courses and computational chemistry infrastructure*, BoRSF Enhancement Grant, \$31,450.
- 2002-03 *Integrating physical chemistry and biology in research and education* (with Donald T. Haynie), BoRSF Enhancement Grant, \$47,500.
- 2003-04 *Bionanotechnology modeling and simulations* (with Donald T. Haynie), BoRSF Enhancement Grant, \$20,000.
- 2004-07 *IMR: Acquisition of a SGI Origin350 for Nano/Bio-Technology Computational Research and Student Training* [with Daniela Mainardi (PI), Andre Paun, and Donald T. Haynie], National Science Foundation, \$119,649. [DMR-0414903]
- 2004-08 *Superior Graduate Fellows in Molecular Science and Nanotechnology* (with William J. Campbell), BoRSF Graduate Fellows Grant, \$72,000.
- 2007-11 *Superior Graduate Students in Engineering* (Scott Gold, PI), BoRSF Graduate Fellows Grant, \$96,000.
- 2007-11 *Doctoral Diversity in Engineering and Sciences at Louisiana Tech University* (Terry McConathy, PI), BoR/SREB Graduate Fellowships, \$190,000.
- 2007-12 *The LONI Institute: Advancing Biology, Materials, and Computational Sciences for Research, Education, and Economic Development*, BoR/Post-Katrina Support Fund Initiative (PI: Mark Jarrell at LSU) \$7.00 M (Role: Science Leader from Louisiana Tech University; LA Tech's share = \$1.28M)
- 2008-09 *Acquisition of Differential Scanning Calorimeters for Undergraduate and Graduate Laboratories and Research*, BoRSF Enhancement Grant, [with Frank Ji (PI), Scott Gold, Tabbetha Dobbins, and Upali Siriwardane] \$57,100.
- 2008-11 *International Chemistry Research Experiences for Students in Vietnam*, National Science Foundation (OISE – Global Scientists & Engineers), L. M. Pratt (PI), Allan R. Pinhas (Co-PI), \$150,000. [OISE-0744375]
- 2008-13 *Superior Graduate Fellows in Biomedical Engineering*, BoRSF Graduate Fellows Grant, \$200,000.
- 2008-13 *Superior Graduate Fellows in Engineering*, BoRSF Graduate Fellows Grant, \$100,000.
- 2009-14 *Graduate Fellows in Biomedical Engineering*, (Steven A. Jones, PI), BoRSF Graduate Fellows Grant, \$100,000.
- 2009-14 *Superior Graduate Fellows Supporting Three Centers of Excellence in Engineering*, (Jim Palmer, PI), BoRSF Graduate Fellows Grant, \$100,000.
- 2010-15 *Graduate Fellows in Engineering 2011-15* (Jim Palmer, PI), BoRSF Graduate Fellows Grant, \$200,000.
- 2010-15 *Graduate Fellows in Computational Analysis and Modeling 2011-15*, BoRSF Graduate Fellows Grant, \$200,000.

- 2010-15 *Louisiana EPSCoR Research Infrastructure Improvement* (Michael Khonsari, PI), National Science Foundation, \$20,000,000. EPS-1003897.
- 2011 *Removal of Trace Water from Cooking Oils*, Frymaster Corporation, \$50,000 (January-June, 2011).
- 2011-12 *Shared Memory Computational Infrastructure for Computational Chemistry and Materials Science Education*, BoRSF Graduate Fellows Grant, \$68,599.
- 2011-16 *Superior Graduate Fellows Supporting Three Centers of Excellence in Engineering*, (Jim Palmer, PI), BoRSF Graduate Fellows Grant, \$300,000.
- 2011-16 *Graduate Fellows in Computational Analysis and Modeling 2011-16*, BoRSF Graduate Fellows Grant, \$200,000.
- 2011-12 *Computational and experimental investigations of the reversible reactions of lithium with nanostructured RuO<sub>2</sub> as potential lithium ion battery anode materials* (Lamar Meda, PI) LA EPSCoR \$34,000.
- 2012-16 *Increasing Diversity in Doctoral Populations at Louisiana Tech University* (Terry McConathy, PI), BoRSF/SREB Doctoral Diversity, \$190,000.
- 2012-17 *Biomedical Engineering Doctoral Graduate Fellows 2013-17* (Steve Jones, PI), BoRSF Graduate Fellows Grant, \$100,000.
- 2012-17 *Superior Graduate Fellows Supporting Five Centers of Excellence in Engineering 2013-2017* (James Palmer, PI), BoRSF Graduate Fellows Grant, \$200,000.
- 2014-19 *Computational Analysis and Modeling Doctoral Graduate Fellows 2015-19* (Weizhong Dai, PI), BoRSF Graduate Fellows Grant, \$100,000.
- 2014-18 *Increasing Diversity in the Doctoral Student Populations at Louisiana Tech University 2014-18* (Sheryl Shoemaker, PI), BoRSF/SREB Doctoral Diversity, \$190,000.
- 2015-19 *Increasing Diversity in the Doctoral Student Populations at Louisiana Tech University 2015-19* (Sheryl Shoemaker, PI), BoRSF/SREB Doctoral Diversity, \$95,000.
- 2015-20 *Superior Graduate Fellows in Molecular Sciences and Nanotechnology 2015-20*, BoRSF Graduate Fellows Grant, \$100,000.
- 2015-20 *RII Track-1: Louisiana Consortium for Innovation in Manufacturing and Materials* (Michael Khonsari, PI), National Science Foundation, \$20,000,000. OIA-1541079.
- 2016-21 *Superior Graduate Fellows in Molecular Sciences and Nanotechnology 2016-21*, BoRSF Graduate Fellows Grant, \$100,000.
- 2016-20 *Increasing Diversity in the Doctoral Student Populations at Louisiana Tech University 2016-20* (Sheryl Shoemaker, PI), BoRSF/SREB Doctoral Diversity, \$95,000.
- 2017-22 *Superior Graduate Fellows in Molecular Sciences and Nanotechnology 2017-22*, BoRSF Graduate Fellows Grant, \$108,000.



- 2017-21 *Increasing Diversity in the Doctoral Student Populations at Louisiana Tech University 2017-21* (Sheryl Shoemaker, PI), BoRSF/SREB Doctoral Diversity, \$95,000.
- 2017-22 *Superior Graduate Fellows Supporting Five Centers of Excellence in Engineering 2017-2022* (James Palmer, PI), BoRSF Graduate Fellows Grant, \$108,000.
- 2018-22 *Increasing Diversity in the Doctoral Student Populations at Louisiana Tech University 2018-21*, BoRSF/SREB Doctoral Diversity, \$90,000
- 2019-23 *Increasing Diversity in the Doctoral Student Populations at Louisiana Tech University 2019-22*, BoRSF/SREB Doctoral Diversity, \$45,000
- 2020-24 *Increasing Diversity in the Doctoral Student Populations at Louisiana Tech University 2020-23*, BoRSF/SREB Doctoral Diversity, \$90,000

## SCIENTIFIC PUBLICATIONS

### A. Articles (Peer-reviewed)

1. B. Ramachandran and Kenneth G. Kay, "Semiclassical Ergodic Properties of the Henon-Heiles System," *Journal of Chemical Physics* **83**, 6316 (1985).
2. B. Ramachandran and Kenneth G. Kay, "Local Ergodicity as a Probe for Chaos in Quantum Systems: Application to the Henon-Heiles System," *Journal of Chemical Physics* **86**, 4628 (1987).
3. Kenneth G. Kay and B. Ramachandran, "Classical and Quantum Pseudoergodic Regions of the Henon-Heiles System," *Journal of Chemical Physics* **88**, 5688 (1988).
4. B. Ramachandran, T.-G. Wei, and Robert E. Wyatt, "The Relative Performances of the Kohn, Schwinger and Newton Variational Principles in Scattering Theory," *Journal of Chemical Physics* **89**, 6785 (1988).
5. B. Ramachandran, T.-G. Wei, and Robert E. Wyatt, "The Role of Basis Set Expansions in the Relative Performances of the Schwinger and Newton Variational Principles," *Chemical Physics Letters* **151**, 540 (1988).
6. B. Ramachandran and Robert E. Wyatt, "How Variational Principles in Scattering Theory Work," in *Supercomputer Algorithms for Reactivity, Dynamics and Kinetics of Small Molecules*, NATO ASI Series, Ed. A. Lagana (Kluwer Academic Publishers, Holland, 1989).
7. B. Ramachandran and R.E. Wyatt, "The Schwinger and the Newton Variational Principles for the Log-Derivative Matrix," *Journal of Chemical Physics* **91**, 1096 (1989).
8. B. Ramachandran and Kenneth G. Kay, "Semiclassical Expectation Values By Adiabatic Switching: Trapping and Tunneling in the Chaotic Regime," *Physical Review A* **41**, 1757 (1990).
9. B. Ramachandran, Michael D'Mello and Robert E. Wyatt, "The Newton Variational Functional for the Log-Derivative Matrix: Use of the Reference Energy Green's Function in an Exchange Problem," *Journal of Chemical Physics* **93**, 8110 (1990).

10. B. Ramachandran and K.G. Kay, "The influence of classical resonances on quantum energy levels," *Journal of Chemical Physics* **99**, 3659 (1993).
11. X. Wu, B. Ramachandran and R.E. Wyatt, "A single arrangement variational method for total reaction probabilities," *Chemical Physics Letters* **214**, 118 (1993).
12. X. Wu, B. Ramachandran and R.E. Wyatt, "A single arrangement variational method for reactive scattering: total and state-resolved reaction probabilities," *Journal of Chemical Physics* **101**, 9395 (1994).
13. B. Ramachandran, "MOBY Molecular Modelling on the P.C, Version 1.5," software review, *Journal of Chemical Education* **71**, A289 (1994).
14. B. Ramachandran, X. Wu and R.E. Wyatt, "A single arrangement variational method for quantum mechanical reactive scattering calculations," in *Toward Teraflop Computing and New Grand Challenge Applications*, R.K. Kalia and P. Vashishta (Eds.), Nova Science, Commack, NY, 1995.
15. B. Ramachandran and P.C. Kong, "Three-dimensional graphical visualization of one electron atomic orbitals," *Journal of Chemical Education* **72**, 406 (1995).
16. B. Ramachandran, "Examining the shapes of atomic orbitals using Mathcad," *Journal of Chemical Education* **72**, 1082 (1995).
17. B. Ramachandran, J. Senekowitsch and R.E. Wyatt, "A new potential surface for the reaction  $O(^3P) + HCl(X^1\Sigma^+) \rightarrow OH(X^2\Pi) + Cl(^2P)$ ," *Journal of Molecular Structure (THEOCHEM)* **388**, 57 (1996). [Special issue in memory of Jan Almlöf.]
18. B. Ramachandran, J. Senekowitsch and R.E. Wyatt, "A quasiclassical trajectory study of the reaction  $O(^3P) + HCl(v=2, j=1,6,9) \rightarrow OH(v',j') + Cl$  on a new potential surface," *Chemical Physics Letters* **270**, 387-394 (1997).
19. T.C. Allison, B. Ramachandran, J. Senekowitsch, D.G. Truhlar, and R.E. Wyatt, "Variational Transition State Theory Calculations of Thermal Rate Coefficients for the  $O(^3P) + HCl$  Reaction," *Journal of Molecular Structure (THEOCHEM)* **454**, 307 (1998).
20. H. Zhang, B. Ramachandran, J. Senekowitsch, and R.E. Wyatt, "Determination of the spectroscopic constants and anharmonic forcefields for HOCl and DOCl using Scaled External Correlation," *Journal of Molecular Structure (THEOCHEM)* **487**, 75 (1999).
21. B. Ramachandran, E.A. Schrader III, J. Senekowitsch, and R.E. Wyatt, "Dynamics of the  $O(^3P) + HCl$  reaction on the  $^3A''$  electronic state: A new *ab initio* potential energy surface, quasi-classical trajectory study, and comparison to experiment," *Journal of Chemical Physics* **111**, 3862 (1999).
22. B. Ramachandran, "Energy disposal in the  $O(^3P) + HCl$  reaction: Classical dynamics and comparison to experiment," *Journal of Chemical Physics* **112**, 3680-3688 (2000).
23. K. Nobusada, H. Nakamura, Y. Lin, and B. Ramachandran, "Quantum reaction dynamics of  $O(^3P) + HCl$  on a new *ab initio* potential energy surface," *Journal of Chemical Physics* **113**, 1018-1026 (2000).
24. B. Ramachandran, N. Balakrishnan, and A. Dalgarno, "Vibrational-rotational distributions of NO formed from  $N + O_2$  reactive collisions," *Chemical Physics Letters* **332**, 562-568 (2000).

25. Y. Lin, B. Ramachandran, K. Nobusada, and H. Nakamura, "Quantum-classical correspondence in the  $O(^3P) + HCl$  and  $Cl(^2P) + OH$  reactions for total angular momentum  $J = 0$ ," *Journal of Chemical Physics* **114**, 1549-1558 (2001).
26. S. Skokov, S. Zou, J. M. Bowman, T. C. Allison, D. G. Truhlar, Y. Lin, B. Ramachandran, B. C. Garrett, and B. J. Lynch, "Thermal and state-selected rate coefficients for the  $O(^3P) + HCl$  reaction and new calculations for the barrier height and width," *Journal of Physical Chemistry A* **105**, 2298-2307 (2001).
27. L. M. Pratt, B. Ramachandran, J. D. Xidos, C. J. Cramer, and D. G. Truhlar, "Structures and Aggregation States of Fluoromethylithium and Chloromethylithium Carbenoids in the Gas Phase and in Ethereal Solvent," *Journal of Organic Chemistry* **67**, 7607-7612 (2002).
28. B. Ramachandran, N. Vegesna, and K. A. Peterson, "Effects of electron correlation and scalar relativistic corrections on the thermochemical and spectroscopic properties of HOF," *Journal of Physical Chemistry A* **107**, 7938-7944 (2003).
29. B. Ramachandran and K. A. Peterson, "Potential energy surfaces for the  $^3A''$  and  $^3A'$  electronic states of the  $O(^3P) + HCl$  system," *J. Chem. Phys.* **119**, 9590-9600 (2003).
30. T. Xie, J.M. Bowman, B. Ramachandran, K. A. Peterson, "Quantum calculations of the rate constant for the  $O(^3P) + HCl$  reaction on new  $^3A''$  and  $^3A'$  surfaces," *J. Chem. Phys.* **119**, 9601-9608 (2003).
31. T. Xie, J.M. Bowman, J. W. Duff, M. Braunstein, and B. Ramachandran, "Quantum and quasiclassical studies of the  $O(^3P) + HCl \rightarrow OH + Cl(^2P)$  reaction using benchmark potential surfaces," *J. Chem. Phys.* **122**, 014301 (2005).
32. L. Pratt, N.V. Nguyễn, and B. Ramachandran, "Computational strategies for evaluating barrier heights for gas phase reactions of lithium enolates," *Journal of Organic Chemistry* **70**, 4279-4283 (2005) .
33. H. F. Ji, Y. Zhang, V. V. Purushotham, S. Kondu, B. Ramachandran, T. Thundat, and D. T. Haynie, "1,6-Hexanedithiol monolayer as a receptor for specific recognition of alkylmercury," *The Analyst*, **130**,1577-1579 (2005).
34. L. M. Pratt and B. Ramachandran, "A computational study of oxiranyllithium," *Journal of Organic Chemistry* **70**, 7238-7242 (2005).
35. B. Ramachandran, "Scaling dynamical correlation energy from Density Functional Theory correlation functions," *Journal of Physical Chemistry A (Donald G. Truhlar Festschrift)* **110**, 396-403 (2006).
36. L. Pasumansky, C. J. Collins, L. M. Pratt, N.V. Nguyễn, B. Ramachandran, and B. Singaram, "Solvent and temperature effects on the reduction and amination reactions of electrophiles by lithium dialkylaminoborohydrides," *Journal of Organic Chemistry* **72**, 971-976 (2007).
37. M. M. Ghouri, S. Singh, and B. Ramachandran, "Scaled Density Functional Theory Correlation Functionals," *Journal of Physical Chemistry A. (Robert E. Wyatt Festschrift)* **111**, 10390-10399 (2007). [#16 most-downloaded paper for third quarter of 2007.]
38. J. D. Nelson, J. Carpenter, S. A. Napper, and B. Ramachandran, "Innovative Administration Supports Innovative Education," *Proceedings of the 38th ASEE/IEEE Frontiers in Education*

(FIE) Conference, Saratoga Springs, NY; October 22-25, art. no. 4720387, pp. T2G3-T2G8 (2008).

39. L. M. Pratt, T. Phuong, N. V. Nguyễn, and B. Ramachandran, "Halomethylithium carbenoid cyclopropanation reactions: A computational study of the effects of solvation and aggregation," *Bulletin of the Chemical Society of Japan* **82**, 1107-1125 (2009).
40. B. Ramachandran, P. Kharidehal, L. M. Pratt, S. Voit, F. N. Okeke, and M. Ewan, "Computational strategies for reactions of aggregated and solvated organolithium carbenoids," *Journal of Physical Chemistry A* **114**, 8423-8433 (2010).
41. G. L. Gutsev, C. A. Weatherford, P. Jenna, E. Johnson, and B. R. Ramachandran, "Structural Patterns in Carbon Chemisorption on an Icosahedral Iron Cluster," *Journal of Physical Chemistry C* **116**, 7050-7061 (2012) DOI: [10.1021/jp300403p](https://doi.org/10.1021/jp300403p)
42. G. L. Gutsev, C. A. Weatherford, P. Jenna, E. Johnson, and B. R. Ramachandran, "Correction to Structural Patterns in Carbon Chemisorption on an Icosahedral Iron Cluster," *Journal of Physical Chemistry C* **116**, 10438 (2012). DOI: [10.1021/jp303534y](https://doi.org/10.1021/jp303534y)
43. B. Ramachandran and Lawrence M. Pratt, "Computational perspectives on organolithium carbenoids," in *Practical Aspects of Computational Chemistry II: An Overview of the Last Two Decades and Current Trends*, Chapter 13, pp. 471-510, Eds. J. Leszczynski, M. K. Shukla, and H. de Rode, Springer, Dordrecht, 2012. [Invited book chapter]
44. G.L. Gutsev, C. A. Weatherford, P. Jena, E. Johnson, and B. R. Ramachandran, "Structure and properties of  $Fe_n$ ,  $Fe_n^-$ , and  $Fe_n^+$  clusters,  $n = 7 - 20$ ," *Journal of Physical Chemistry A* **116**, 10218-10228 (2012); DOI: [10.1021/jp307284v](https://doi.org/10.1021/jp307284v)
45. L.M. Pratt, B. K. Mai, and B.R. Ramachandran, "Carbenoid alkene insertion reactions of oxiranyllithiums," *Journal of Organic Chemistry* **77**, 8605-8614 (2012). DOI: [10.1021/jo301550y](https://doi.org/10.1021/jo301550y)
46. B. R. Ramachandran, S. D. Baker, G. Suravajhula, and P. Derosa, "Selective complexation of alkali metal ions using crown ethers derived from calix[4]arenes: A computational investigation of the structural and energetic factors," *Journal of Inclusion Phenomena and Macrocyclic Chemistry* **75**, 185-195 (2013) (published on-line June 9, 2012) DOI: [10.1007/s10847-012-0160-6](https://doi.org/10.1007/s10847-012-0160-6)
47. G. L. Gutsev, C. A. Weatherford, P. Jena, and B. R. Ramachandran, "Competition between surface chemisorption and cage formation in  $Fe_{12}O_{12}$  clusters," *Chemical Physics Letters* **556**, 211-216 (2013). DOI: [10.1016/j.cplett.2012.11.054](https://doi.org/10.1016/j.cplett.2012.11.054)
48. G. L. Gutsev, C. A. Weatherford, K. G. Belay, B. R. Ramachandran, "An all-electron density functional theory study on the structure and properties of the neutral and singly charged  $M_{12}$  and  $M_{13}$  clusters:  $M=Sc-Zn$ ," *Journal of Chemical Physics* **138**, 164303 (2013). DOI: [10.1063/1.4799917](https://doi.org/10.1063/1.4799917)
49. B. R. Ramachandran, S. M. Waithe, and L. M. Pratt, "Rearrangement reactions of lithiated oxiranes," *Journal of Organic Chemistry* **78**, 10776-10783 (2013). DOI: [10.1021/jo401763v](https://doi.org/10.1021/jo401763v)
50. B. R. Ramachandran, S. M. Waithe, and L. M. Pratt, "Correction to: Rearrangement reactions of lithiated oxiranes," *Journal of Organic Chemistry* **79**, 471-471 (2014). DOI: [10.1021/jo4026397](https://doi.org/10.1021/jo4026397)

51. L.M. Pratt, B. K. Mai, and B.R. Ramachandran, "Correction to: Carbenoid alkene insertion reactions of oxiranyllithiums," *Journal of Organic Chemistry* **79**, 472-472 (2014). DOI: [10.1021/jo4026572](https://doi.org/10.1021/jo4026572)
52. G.L. Gutsev, L. E. Johnson, K. G. Belay, C. A. Weatherford, L. L. Gutsev, and B. R. Ramachandran, "Structure and magnetic properties of Fe<sub>12</sub>X clusters," *Chemical Physics* **430**, 62-68 (2014). DOI: [10.1016/j.chemphys.2013.12.014](https://doi.org/10.1016/j.chemphys.2013.12.014)
53. G. L. Gutsev, L. E. Johnson, K. G. Belay, C. A. Weatherford, L. G. Gutsev, B. R. Ramachandran, "Structure and magnetic properties of Fe<sub>n</sub>Gd clusters, *n* = 12 -19," *European Physical Journal D* **68**, 81 (9 pages) (2014). DOI: [10.1140/epjd/e2014-40830-3](https://doi.org/10.1140/epjd/e2014-40830-3)
54. A. S. Hassan, A. Navulla, L. Meda, B. R. Ramachandran, and C. D. Wick, "Molecular Mechanisms for the Lithiation of Ruthenium Oxide (RuO<sub>2</sub>) Nanoplates as Lithium-Ion Battery Anode Materials: An Experimentally Motivated Computational Study," *Journal of Physical Chemistry C*, **119**, 9705-9713 (2015). DOI: [10.1021/jp5123536](https://doi.org/10.1021/jp5123536)
55. G. L. Gutsev, K. G. Belay, C. A. Weatherford, B. R. Ramachandran, L. G. Gutsev, and P. Jena, "Structure and magnetic properties of polyfluoride F<sub>n</sub><sup>-</sup> clusters (*n* = 3-29)," *Journal of Physical Chemistry A*, **119**, 6483-6492 (2015). DOI: [10.1021/acs.jpca.5b02431](https://doi.org/10.1021/acs.jpca.5b02431)
56. G. L. Gutsev, C. A. Weatherford, B. R. Ramachandran, L. G. Gutsev, W.-J. Zheng, O. C. Thomas, and K. H. Bowen, "Photoelectron spectra and structure of the Mn<sub>n</sub><sup>-</sup> anions (*n* = 2 – 16)," *Journal of Chemical Physics*, **143**, 044306 (2015). DOI: [10.1063/1.4926943](https://doi.org/10.1063/1.4926943)
57. L.G. Gutsev, N. S. Dalal, B. Ramu Ramachandran, C. A. Weatherford, and G. L. Gutsev, "Spectral signatures of semiconductor clusters: (CdSe)<sub>16</sub> isomers," *Chem. Phys. Lett.* **636**, 121-128 (2015). DOI: [10.1016/j.cplett.2015.07.024](https://doi.org/10.1016/j.cplett.2015.07.024)
58. A. S. Hassan, K. Moyer, B. R. Ramachandran, and C. D. Wick, "Comparison of Storage Mechanisms in RuO<sub>2</sub>, SnO<sub>2</sub>, and SnS<sub>2</sub> for Lithium-Ion Battery Anode Materials," *J. Phys. Chem. C* **120**, 2036–2046 (2016). DOI: [10.1021/acs.jpcc.5b09078](https://doi.org/10.1021/acs.jpcc.5b09078)
59. S. B. Ranganath, S. Hartman, A. S. Hassan, C. D. Wick, and B. R. Ramachandran, "Interfaces in Metal, Alloy, and Metal Oxide Anode Materials for Lithium Ion Batteries," in *Proceedings of the 3rd Annual Conference on Materials Science, Metals, and Manufacturing (M3)*, pp. 83-87, Global Science and Technology Forum, Singapore, 2016. DOI: [10.5176/2251-1857\\_M316.28](https://doi.org/10.5176/2251-1857_M316.28)
60. S. B. Ranganath, A. S. Hassan, B. R. Ramachandran and Collin D. Wick, "Role of Metal-Lithium Oxide Interfaces in the Extra Lithium Capacity of Metal Oxide Lithium-Ion Battery Anode Materials," *J. Electrochem. Soc.*, **163**, A2172-A2178 (2016). DOI: [10.1149/2.0281610jes](https://doi.org/10.1149/2.0281610jes)
61. G. L. Gutsev, K. G Belay, L. G. Gutsev and B. R. Ramachandran, "Structure and Properties of Iron Oxide Clusters: from Fe<sub>6</sub> to Fe<sub>6</sub>O<sub>20</sub> and from Fe<sub>7</sub> to Fe<sub>7</sub>O<sub>24</sub>," *J. Comp. Chem.*, **37**, 2527-2536 (2016). DOI: [10.1002/jcc.24478](https://doi.org/10.1002/jcc.24478)
62. M. Ferdows, D. Liu, and B. R. Ramachandran, "Boundary Layer Slip and Heat Transfer in Stagnation Point Flow over a Steady Stretching Surface Embedded in a Porous Medium with Heat Sources," *British J. Math. & Comp. Sci.* **18**, BJMCS.28212 (2016). DOI: [10.9734/BJMCS/2016/28212](https://doi.org/10.9734/BJMCS/2016/28212)

63. G. L. Gutsev, B. R. Ramachandran, L. G. Gutsev, and K. V. Bozhenko, "A comparative study of the 3d-metal oxide clusters (FeO)<sub>n</sub>, (CoO)<sub>n</sub>, and (NiO)<sub>n</sub>, (n = 1-10)," *Phys. Chem. Chem. Phys.* **18**, 27858-27867 (2016). DOI: [10.1039/c6cp03241a](https://doi.org/10.1039/c6cp03241a)
64. M. Ferdows, D. Liu, and B. R. Ramachandran, "02-D Magnetohydrodynamics Boundary Layer Flow of Cu-Ag-TiO<sub>3</sub>-Al<sub>2</sub>O<sub>3</sub>-H<sub>2</sub>O-C<sub>2</sub>H<sub>6</sub>O<sub>2</sub> Mixtures: Explicit Numerical and Stability Approach," *J. Mod. Mech. Engr. and Technol.* **3**, 41-59 (2016). E-ISSN: 2409-9848/16.
65. B. R. Ramachandran, S. Sun, C. D. Wick, "Oxidation of iron and iron-chromium surfaces: Preliminary results from computational studies," in *Proceedings of the 4th Annual Conference on Materials Science, Metals, and Manufacturing (M3)*, pp. 46-52, Global Science and Technology Forum, Singapore, 2017. DOI: [10.5176/2251-1857\\_M317.20](https://doi.org/10.5176/2251-1857_M317.20)
66. G. L. Gutsev, K. G. Belay, L. G. Gutsev, and B. R. Ramachandran "Geometrical and magnetic structure of iron oxide clusters (FeO)<sub>n</sub> for n > 10," *Computational Materials Science.* **137**, 134-143 (2017). DOI: [10.1016/j.commatsci.2017.05.028](https://doi.org/10.1016/j.commatsci.2017.05.028)
67. X. Zhang, B. Zhang, Y. Mu, S. Shao, C. D. Wick, B. R. Ramachandran, and W. J. Meng, "On failure of ceramic/metal/substrate interfacial regions under shear loading," *Acta Materialia* **138**, 224-236 (2017), DOI: [10.1016/j.actamat.2017.07.053](https://doi.org/10.1016/j.actamat.2017.07.053)
68. S. Sun, B. R. Ramachandran, and C.D. Wick, "Solid, Liquid, and Interfacial Properties of TiAl Alloys: Parameterization of a New Modified Embedded Atom Method Model," *Journal of Physics: Condensed Matter* **30**, 075002 (2018). DOI: [10.1088/1361-648X/aaa52c](https://doi.org/10.1088/1361-648X/aaa52c)
69. G. L. Gutsev, K. G. Belay, L. G. Gutsev, B. R. Ramachandran, and P. Jena, "Effect of Hydrogenation on the Structure and Magnetic Properties of an Iron Oxide Cluster," *Phys. Chem. Chem. Phys.* **20**, 4546-4553 (2018), DOI: [10.1039/C7CP08224J](https://doi.org/10.1039/C7CP08224J)
70. L. G. Gutsev, B. R. Ramachandran, and G. L. Gutsev, "Pathways of Growth of CdSe Nanocrystals from Nucleant (CdSe)<sub>34</sub> Clusters," *Journal of Physical Chemistry C*, **122**, 3168-3175 (2018), DOI: [10.1021/acs.jpcc.7b12716](https://doi.org/10.1021/acs.jpcc.7b12716)
71. S. B. Ranganath, C. D. Wick, and B. R. Ramachandran, "Role of structure and oxidation states in the passivation of stainless steel by chromium," in *Proceedings of the 8<sup>th</sup> Annual International Conference on Sustainable Energy and Environmental Sciences (SEES 2019)*, pp. 10-13, Global Science and Technology Forum, Singapore, 2019. DOI: [10.5176/2251-189X\\_SEES19.65](https://doi.org/10.5176/2251-189X_SEES19.65)
72. A. S. M. Miraz, S. Sun, S. Shao, W. J. Meng, B. R. Ramachandran, and C.D. Wick, "Computational Study of Metal/Ceramic Interfacial Adhesion and Barriers to Shear Displacement," *Computational Materials Science* **168**, 104-115 (2019). DOI: [10.1016/j.commatsci.2019.06.006](https://doi.org/10.1016/j.commatsci.2019.06.006)
73. P. R. Albuquerque, B. R. Ramachandran, T. Junk, and T. N. V. Karsili, "Hydrogen-Deuterium Exchange in Basic Near-Critical and Supercritical Media: An Experimental and Theoretical study," *Journal of Physical Chemistry A* **124**, 2530-2536 (2020). DOI: [10.1021/acs.jpca.9b10892](https://doi.org/10.1021/acs.jpca.9b10892)
74. A. Boldyreva, L. Frolova, I. Zhidkov, L. Gutsev, E. Kurmaev, B. R. Ramachandran, V. Petrov, K. Stephenson, S. Aldoshin, P. Troshin, "Unravelling the Material Composition Effects on the Gamma Ray Stability of Lead Halide Perovskite Solar Cells: MAPbI<sub>3</sub> Breaks

- the Records,” *Journal of Physical Chemistry Letters* **11**, 2630-2636 (2020). DOI: [10.1021/acs.jpcllett.0c00581](https://doi.org/10.1021/acs.jpcllett.0c00581)
75. A. S. M. Miraz, E. Williams, W. J. Meng, B. R. Ramachandran, and C. D. Wick, “Improvement of Interfacial Shear Strength of Ti/TiN Nanolaminates by Doping– A First Principles Density Functional Theory Study,” *Applied Surface Science* **517**, 146185 (2020). DOI: [10.1016/j.apsusc.2020.146185](https://doi.org/10.1016/j.apsusc.2020.146185)
76. G. L. Gutsev, H. A. López Peña, S. L. McPherson, D. A. Boateng, B. R. Ramachandran, L. G. Gutsev, and K. M. Tibbetts, “From Neutral Aniline to Aniline Trication: A Computational and Experimental Study,” *Journal of Physical Chemistry A* **124**, 3120-3134 (2020). DOI: [10.1021/acs.jpca.0c00686](https://doi.org/10.1021/acs.jpca.0c00686)
77. S. Bhasker-Ranganath, C. D. Wick, and B. R. Ramachandran, “Computational Insights into the Molecular Mechanisms for Chromium Passivation of Stainless-steel Surfaces,” *Materials Today Chemistry* **17**, 100298 (2020). DOI: [10.1016/j.mtchem.2020.100298](https://doi.org/10.1016/j.mtchem.2020.100298)
78. X. Zhang, S. Shao, A. S. M. Miraz, C.D. Wick, B.R. Ramachandran, W.J. Meng, “Low temperature growth of Cu thin films on TiN(001) templates: Structure and Energetics,” *Materialia* **12**, 100748 (2020). DOI: [10.1016/j.mtla.2020.100748](https://doi.org/10.1016/j.mtla.2020.100748)
79. G. L. Gutsev, S. L. McPherson, H. A. López Peña, D. A. Boateng, L. G. Gutsev, B. R. Ramachandran, and K. M. Tibbetts, “Dissociation of Singly and Multiply Charged Nitromethane Cations: Femtosecond Laser Mass Spectrometry and Theoretical Modeling,” *Journal of Physical Chemistry A*, **124**, 7427-7438 (2020). DOI: [10.1021/acs.jpca.0c06545](https://doi.org/10.1021/acs.jpca.0c06545)
80. A. S. M. Miraz, N. Dhariwal, W. J. Meng, B. R. Ramachandran, and Collin D. Wick, “Development and application of interatomic potentials to study the stability and shear strength of Ti/TiN and Cu/TiN interfaces,” *Materials & Design*, **196**, 109123 (2020). DOI: [10.1016/j.matdes.2020.109123](https://doi.org/10.1016/j.matdes.2020.109123)
81. B. Chen, G. L. Gutsev, W. Sun, X. Kuang, C. Lu, L. G. Gutsev, B. R. Ramachandran, S. M. Aldoshin, “Dissociation of dinitrogen on iron clusters: A detailed study of the  $\text{Fe}_{16} + \text{N}_2$  case,” *Physical Chemistry Chemical Physics*, **23**, 2166-12178 (2021) DOI: [10.1039/D0CP05427E](https://doi.org/10.1039/D0CP05427E)
82. A.A. Parfenov, O. R. Yamilova, L. G. Gutsev, D. K. Sagdullina, A. V. Navikov, B. R. Ramachandran, K. J. Stephenson, S. M. Aldoshin, P. A. Troshin, “Highly sensitive and selective ammonia gas sensor based on  $\text{FAPbCl}_3$  lead halide perovskite,” *Journal of Materials Chemistry C*, to be published, 2021. DOI: [10.1039/D0TC03559A](https://doi.org/10.1039/D0TC03559A)
83. A. F. Akbulatov, M. I. Ustinova, L. Gutsev, B. R. Ramachandran, S. A. Tsarev, N. N. Dremova, I. Zhidkov, S. Yu. Luchkin, E. Z. Kurmaev, K. J. Stevenson, S. M. Aldoshin, and P. A. Troshin, “When bromide meets iodide: halide mixing facilitates light-induced decomposition of perovskite absorber films,” *Nano Energy*, submitted, Dec. 2020.
84. A.S.M. Miraz, W. J. Meng, B. R. Ramachandran, and C. D. Wick, “Computational observation of the strengthening of Cu/TiN metal/ceramic interfaces by sub-nanometer interlayers and dopants,” *Applied Surface Science*, submitted, Jan. 2021.
85. N. Dhariwal, A. S. M. Miraz, B. R. Ramachandran, and C. D. Wick, “Computational modeling of Cr/TiN metal/ceramic interface using second nearest-neighbor modified embedded-atom interatomic potential,” in preparation.

## B. Books/Book Chapters

1. Ramachandran and R. E. Wyatt, "How Variational Principles in Scattering Theory Work," in *Supercomputer Algorithms for Reactivity, Dynamics and Kinetics of Small Molecules*, NATO ASI Series, Ed. A. Lagana (Kluwer Academic Publishers, Holland, 1989).
2. B. Ramachandran, X. Wu and R.E. Wyatt, "A single arrangement variational method for quantum mechanical reactive scattering," in *Toward Teraflop Computing and Other Grand Challenge Applications*, Eds. R. Kalia and P. Vashishta, Nova Science, Commack, NY (1995).
3. B. Ramachandran, K. J. Laidler, and J. H. Meiser, *Solutions Manual for "Physical Chemistry"* by K. J. Laidler and J. H. Meiser, 3rd Ed., Houghton-Mifflin, Boston, 1999.
4. B. Ramachandran, *Solutions Manual for "Physical Chemistry"* by K. J. Laidler, J. H. Meiser, and B. C. Sanctuary, 4th Ed., Houghton-Mifflin, Boston, 2002.
5. B. Ramachandran and Lawrence M. Pratt, "Computational perspectives on organolithium carbenoids," in *Practical Aspects of Computational Chemistry II: An Overview of the Last Two Decades and Current Trends*, Eds. J. Leszczynski, M. K. Shukla, and H. de Rode, Springer, Dordrecht, 2012.

## C. Technical Reports

1. T.C. Allison, B. Ramachandran, J. Senekowitsch, D.G. Truhlar, and R.E. Wyatt, "Variational Transition State Theory Calculations of Thermal Rate Coefficients for the  $O(^3P) + HCl$  Reaction," Research Report of the Minnesota Supercomputer Institute, MSI 1998/81.
2. S. Skokov, S. Zou, J. M. Bowman, T. C. Allison, D. G. Truhlar, Y. Lin, B. Ramachandran, B. C. Garrett, and B. J. Lynch, "Thermal and state-selected rate coefficients for the  $O(^3P) + HCl$  reaction and new calculations for the barrier height and width," Research Report of the Minnesota Supercomputer Institute, MSI 2000/235.
3. L. M. Pratt, B. Ramachandran, J. D. Xidos, C. J. Cramer, and D. G. Truhlar, "Structures and Aggregation States of Fluoromethylithium and Chloromethylithium Carbenoids in the Gas Phase and in Ethereal Solvent," UMSI 2002/196.

## SELECTED CONFERENCE PRESENTATIONS

- "Mechanical Failure of Metal/Ceramic Interfaces: A Combined Experimental and Simulation Study," X. Zhang, Y. Mu, M. Dodaran, S. Shao, W.J. Meng, C.D. Wick, and B.R. Ramachandran, IUTAM Symposium on Size-effect in Microstructure and Damage Evolution, Copenhagen, May 28-June 1, 2018 (contributed).
- "Mechanical failure of metal/ceramic interfacial regions," X. Zhang, B. Zhang, Y. Mu, S. Shao, C.D. Wick, B.R. Ramachandran, W.J. Meng, Fall 2017 Meeting of the Materials Research Society, Boston, MA, November 26-December 1, 2017 (contributed).
- "Understanding mechanical integrity of metal/ceramic interfaces through in-situ microscale mechanical testing and multiscale modeling and simulations," S. Shao, X. Zhang, B. Zhang,



Y. Mu, C.D. Wick, B.R. Ramachandran, and W.J. Meng, *Materials Science & Technology 2017 (MS&T 17)*, Pittsburgh, PA, October 8-12, 2017 (contributed).

- “Oxidation of iron and iron-chromium surfaces: Preliminary results from computational studies,” at the 4th Annual Conference on Materials Science, Metals, and Manufacturing (M3), Singapore, March 7-8, 2017 (invited).
- “Interfaces in Metal, Alloy, and Metal Oxide Anode Materials for Lithium Ion Batteries,” at the 3rd Annual Conference on Materials Science, Metals, and Manufacturing (M3), Singapore, January 18-19, 2016 (invited).
- “Density functional theory study of lithium ion battery anode materials: Ruthenium (IV) oxide, tin (IV) oxide, and tin (IV) sulfide,” invited talk at 249<sup>th</sup> ACS National Meeting, Denver, CO at the “Computational Chemical Dynamics: Advancing our Understanding of Chemical Processes in Gas-Phase, Biomolecular & Condensed Phases” Symposium in honor of Donald G. Truhlar, March 23, 2015 (invited).
- “Energy Materials Research in LA-SiGMA,” B. Ramachandran, 2012 Technical Meeting of the Center for Atomic-scale Catalyst Design (a DoE EFRC), Baton Rouge, LA, October 8-10, 2012 (invited).
- “Calixarene Crown Ethers and Carbon Cages,” B. Ramachandran, 9<sup>th</sup> Discussion Meeting on Spectroscopy and Dynamics of Molecules and Clusters, Bangalore, India, February 17-19, 2012 (invited).

#### **SELECTED INVITED SEMINARS/TALKS:**

- “Applications of Computational Chemistry to Engineering Problems,” at the South-Eastern Regional Meeting of the American Chemical Society (SERMACS), Symposium on Applications of Computational Chemistry to Interesting Problems, October 21, 2019.
- “Design of Metal/ceramic Interfaces for Engineering Applications,” at the Army ERDC Computational Chemistry Conference, Vicksburg, MS, September 26, 2019.
- “Scientific Research: Opportunities and Threats,” Keynote speech at the Arkansas Undergraduate Research Conference, Henderson State University, Arkadelphia, AR, April 5, 2019.
- “Applications of Computational Chemistry to Engineering Problems,” at the Department of Chemistry, University of Louisiana at Lafayette, LA, February 7, 2019.
- “Computational Investigations of High Capacity Anode Materials for Lithium Ion Batteries,” invited “Mole Day” seminar at Henderson State University, Arkadelphia, AR, October 23, 2015.
- “Research Overview: Consortium for Innovation in Manufacturing and Materials,” at the McCormick College of Engineering, Northwestern University, Evanston, IL, September 25, 2015.
- “Density functional theory study of metal oxide and sulfides as lithium battery anode materials,” invited seminar at University of New Orleans, New Orleans, LA (February 20, 2015).

- “Computational studies of lithium intercalation in ruthenium oxide nanoplates and nanoparticles,” invited seminar at Universidad Nacional de Cordoba, Cordoba, Argentina, June 18, 2013.
- “Computational studies of lithium intercalation in ruthenium oxide nanoplates and nanoparticles,” invited seminar at Universidad de Rio Cuarto, Rio Cuarto, Argentina, June 17, 2013.

## **SERVICE**

### **A. Service to Department/College/University**

- Campus Computing Services Coordinating Committee (1992-present).
- Program Chair of Chemistry (1996-1998).
- Associate of the Leadership Team (1997-1998).
- Mathematics Faculty Search Team (2001-02, 2002-03).
- University Strategic Planning Subcommittee (2001-present)
- Chaired the CEnIT proposal review team, led the effort for reviewing 91 equipment proposals and 37 research proposals. (2001-2002).
- University Catalog Revision Committee (2002-present).
- Graduate Council, (2002-2008).
- Research Council (2002-present)
- Various other service activities on behalf of the College as a member of the Leadership Team (1998-present).
- NCAA Gender Equities Sub-Committee (2006-present)
- Export Control Policies Committee (Aug 2011-present)
- Faculty search teams (multiple, almost every year, including chairing some teams)
- Vice-President for R&D Research Growth Team (2014-present)

### **B. Service to the State of Louisiana**

- Louisiana Optical Network Initiative (LONI) Resource Allocation Committee, member (2006-2014)
- Louisiana Optical Network Initiative (LONI) Resource Allocation Committee, Chair (2014-present)
- Louisiana Optical Network Initiative (LONI) Software Committee, member (2006-present)
- Southern Universities Research Association (SURA) JSA Programs (Jefferson Lab) Committee, member (2008-present)
- Louisiana Optical Network Infrastructure Management Council, UL System Representative (July 2013-present)

### C. Service to Profession (Reviewer)

- Scientific publication referee for the following journals (ongoing)
  - ACS Organometallics*
  - Advanced Theory and Simulations*
  - Atmospheric Environment*
  - Chemical Physics Letters,*
  - Chemical Physics*
  - Computer Physics Communications*
  - Journal of the American Chemical Society*
  - Journal of Chemical Physics*
  - Journal of Computational Chemistry*
  - Journal of Fluorine Chemistry*
  - Journal of Inclusion Phenomena and Macrocyclic Chemistry*
  - Journal of Organometallic Chemistry*
  - Journal of Physical Chemistry A*
  - Journal of Physical Chemistry B*
  - Journal of Physical Chemistry C*
  - Journal of Molecular Structure (THEOCHEM)*
  - Materials Chemistry and Physics*
  - Materials Today Letters*
  - Molecules*
  - New Journal of Chemistry*
  - Physical Chemistry Chemical Physics*
  - Proceedings of the Louisiana Academy of Sciences Structural Chemistry*
- Proposal referee for the following funding organizations (ongoing)
  - American Chemical Society (Petroleum Research Fund).*
  - National Science Foundation (Theoretical and Computational Chemistry Division)*
  - National Science Foundation Graduate Research Fellowship Program (panelist)*