

Bala Ramu Ramachandran

*Hazel Stewart Garner Professor of Chemistry
Associate Dean of Research
College of Engineering and Science
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EDUCATION:

B.Sc., Chemistry, University of Calicut, India, June 1980
MSc., 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-present

ADMINISTRATIVE EXPERIENCE (Reverse Chronological):

July 2008-Present: *Associate Dean for Research*

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-present: *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*

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 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*

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*

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.
- 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.
- 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

SCIENTIFIC/PROFESSIONAL SOCIETIES

American Physical Society (APS)

American Chemical Society (ACS)

American Society for Engineering Education (ASEE)

GRANTS/CONTRACTS:

- 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-
- 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 (Research Subprogram) (Edward Sidel, PI) \$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.

SCIENTIFIC PUBLICATIONS

A. Articles (Peer-reviewed)

1. B. Ramachandran and Kenneth G. Kay, "Semiclassical Ergodic Properties of the Henon-Heiles System," *J. Chem. Phys.* **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," *J. Chem. Phys.* **86**, 4628 (1987).
3. Kenneth G. Kay and B. Ramachandran, "Classical and Quantum Pseudoergodic Regions of the Henon-Heiles System," *J. Chem. Phys.* **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," *J. Chem. Phys.* **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," *Chem. Phys. Lett.* **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," *J. Chem. Phys.* **91**, 1096 (1989).
8. B. Ramachandran and Kenneth G. Kay, "Semiclassical Expectation Values By Adiabatic Switching: Trapping and Tunneling in the Chaotic Regime," *Phys. Rev. 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," *J. Chem. Phys.* **93**, 8110 (1990).
10. B. Ramachandran and K.G. Kay, "The influence of classical resonances on quantum energy levels," *J. Chem. Phys.* **99**, 3659 (1993).
11. X. Wu, B. Ramachandran and R.E. Wyatt, "A single arrangement variational method for total reaction probabilities," *Chem. Phys. Lett.* **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," *J. Chem. Phys.* **101**, 9395 (1994).
13. B. Ramachandran, "MOBY Molecular Modelling on the P.C, Version 1.5," software review, *J. Chem. Educ.* **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," *J. Chem. Educ.* **72**, 406 (1995).
16. B. Ramachandran, "Examining the shapes of atomic orbitals using Mathcad," *J. Chem. Educ.* **72**, 1082 (1995).
17. B. Ramachandran, J. Senekowitsch and R.E. Wyatt, "A new potential surface for the reaction $O(^3P) + HCl(X^1\Sigma^+) \rightarrow OH(X^2\Pi) + Cl(^2P)$," *J. Mol. Struct. (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," *Chem. Phys. Lett.* **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," *J. Mol. Struct. 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," *J. Mol. Struct. 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," *J. Chem. Phys.* **111**, 3862 (1999).
22. B. Ramachandran, "Energy disposal in the $O(^3P) + HCl$ reaction: Classical dynamics and comparison to experiment," *J. Chem. Phys.* **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," *J. Chem. Phys.* **113**, 1018-1026 (2000).
24. B. Ramachandran, N. Balakrishnan, and A. Dalgarno, "Vibrational-rotational distributions of NO formed from $N + O_2$ reactive collisions," *Chem. Phys. Lett.* **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 $J = 0$," *J. Chem. Phys.* **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," *J. Phys. Chem. 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," *J. Org. Chem.* **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," *J. Phys. Chem. 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," *J. Org. Chem.* **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," *J. Org. Chem.* **70**, 7238-7242 (2005).
35. B. Ramachandran, "Scaling dynamical correlation energy from Density Functional Theory correlation functions," *J. Phys. Chem. 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," *J. Org. Chem.* **72**, 971-976 (2007).
37. M. M. Ghouri, S. Singh, and B. Ramachandran, "Scaled Density Functional Theory Correlation Functionals," *J. Phys. Chem. A. (Robert E. Wyatt Festschrift)* **111**, 10390-10399 (2007). [**#16 most-downloaded papers 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," *Bull. Chem. Soc. Japan* **82**, 1107-1125 (2009).
40. B. Ramachandran, Purnima Kharidehal, Lawrence M. Pratt, Stewart Voit, Fabian N. Okeke, and Monique Ewan, "Computational Strategies for Reactions of Aggregated and Solvated Organolithium Carbenoids," *J. Phys. Chem. A* (submitted).
41. S. Vudatha, D. T. Haynie, and B. Ramachandran, "Reaction thermodynamics of methylmercury with thiols in gas and aqueous phases: A computational study," *J. Phys. Chem. A* (to be submitted).
42. P. Alburquerque, T. Junk, and B. Ramachandran, "Calculations of the acidities of n-butylbenzene protons in aqueous media under normal and supercritical conditions," *J. Org. Chem.* (to be submitted).
43. S. A. Baker, B. Ramachandran, and P. Derosa, "Selective Complexation of Alkali Metal Cations with Calix[4]Crowns in Aqueous Media: A Density Functional Theory Study," *J. Mol. Struct. (Theochem)* (work in progress).
44. D. S. Patel, B. Ramachandran, D. Kuila, S. Datta, D. B. Janes, and D. G. Truhlar, "Structure and properties of aromatic thiols and dithiols adsorbed on Au (111) surfaces: A Density Functional Theory Study," *J. Phys. Chem. B* (work in progress).

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.

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.

PRESENTATIONS

(Only invited lectures and recent conference presentations are listed. Coauthors of papers are indicated where applicable.)

- "The Newton variational Method for the log-derivative matrix: Application to atom-molecule reactions," invited seminar at Delta State University, Cleveland, MS (January 1995).
- "A single arrangement method for atom-molecule reactive scattering calculations," invited seminar at Jackson State University, Jackson, MS (January 1995).
- "Dynamics of the $O(^3P) + HCl$ on a new potential energy surface," invited research seminar at University of Texas, Austin, TX (May 1997).
- "Quasiclassical trajectory study of the dynamics of the $O(^3P) + HCl$ reaction," at the XVth Conference on the Dynamics of Molecular Collisions, Brainerd, MN (July 1997).
- "New potential energy surfaces and trajectory dynamics of the $O(^3P) + HCl$ reaction," at the Gordon Research Conference on Atomic and Molecular Interactions, New London, NH (June 1998).

- “Dynamics of the $O(^3P) + HCl$ reaction: Role of the $^3A''$ and $^3A'$ electronic states,” invited lecture at the symposium on “Molecular Structure and Dynamics,” at the 54th ACS South West Regional Meeting, Baton Rouge, LA (Nov. 1-3, 1998), Invited symposium presentation.
- “Dynamics of the $O(^3P) + HCl$ reaction: Role of the $^3A''$ and $^3A'$ electronic states,” at the XVIIth Conference on the Dynamics of Molecular Collisions, Lake Harmony, PA (July 1999).
- “Spectroscopic constants, anharmonic forcefields, and bound states of HOCl and DOCl,” B. Ramachandran and J. A. Bentley, at the XVIIth Conference on the Dynamics of Molecular Collisions, Lake Harmony, PA (July 1999).
- “A computational study of fluoromethylithium and chloromethylithium carbenoids,” L. M. Pratt, D. G. Truhlar, C. J. Cramer, J. D. Xidos, and B. Ramachandran, at the American Chemical Society National Meeting, San Diego, CA (August 1999).
- “Study of an elementary gas phase reaction: Energy disposal and classical dynamics,” invited research seminar at University of Louisiana, Monroe (December 1999).
- “Construction of accurate potential energy surfaces for small molecular systems,” invited lecture to the attendees of the NSF-supported “Computational Chemistry Workshop” at the *Computational Center for Molecular Structure and Interaction*, Jackson State University, Jackson, MS, August 2001.
- “Structure and energetics of halide-bridged binuclear complexes of Ni(II): A computational study,” B. Ramachandran, R. E. Norman, and D. G. Truhlar, at the Xth Conference on Current Trends in Computational Chemistry, Jackson, MS (November 2001).
- “Construction of accurate potential energy surfaces for small molecular systems,” invited lecture at the Indian Institute of Science, Bangalore, India (June 2002).
- “Potential energy surfaces for the $^3A''$ and $^3A'$ electronic states of the $O(^3P) + HCl$ system and calculations of thermal rate constants,” B. Ramachandran, K. A. Peterson, T. Xie, and J. M. Bowman, at the XIth Conference on Current Trends in Computational Chemistry, Jackson, MS (November 2002).
- “Dipole moments of organic thiols on Gold surface,” P. Das, D. Patel, D. Kuila, B. Ramachandran, and D. Janes, 2002 March meeting of the American Physical Society, Austin, TX, March 5-7, 2003.
- “Theoretical Studies on Nanoscale Charge Transfer in Self Assembled Monolayers (SAMs) of Organic Thiols on Gold,” D. S. Patel, P. Das, D. Janes, S. Datta, B. Ramachandran, and D. Kuila, Division of Colloid and Surface Chemistry, 225th ACS National Meeting, New Orleans, LA, March 23-27, 2003.
- “Two explorations: Scaling correlation energy in Density Functional Theory, and Computational studies in organolithium chemistry,” invited seminar at University of Hyderabad, India, November 26, 2007.

- “Two explorations: Scaling correlation energy in Density Functional Theory, and Computational studies in organolithium chemistry,” invited seminar at Indian Institute of Technology, Chennai, India, November 29, 2007.
- “Two explorations: Scaling correlation energy in Density Functional Theory, and Computational studies in organolithium chemistry,” invited seminar at Mississippi College, Clinton, MS, February 4, 2008.
- “Calculations of the acidities of n-butylbenzene protons in aqueous media under normal and supercritical conditions,” P. Albuquerque, T. Junk, and B. Ramachandran, poster presented at the 2008 ACS National Meeting, New Orleans, April 5-8, 2008.
- “Cyclopropanation Reactions of Halomethylithium Carbenoids: A Computational Study of the Effects of Aggregation and Solvation,” 64th South-West Regional Meeting of the American Chemical Society, Little Rock, AR October 6-8, 2008 (Invited talk at the Computational Chemistry Symposium)
- “Calculations of the acidities of n-butylbenzene protons in aqueous media under normal and supercritical conditions,” P. Albuquerque, T. Junk, and B. Ramachandran, poster presented at the 64th South-West Regional Meeting of the American Chemical Society, Little Rock, AR October 6-8, 2008.
- "Selective Complexation of Alkali Metal Cations with Calix[4]Crowns in Aqueous Media: A Density Functional Theory Study" S. A. Baker, B. Ramachandran, and P. Derosa, poster presented at the 64th South-West Regional Meeting of the American Chemical Society, Little Rock, AR October 6-8, 2008.
- "Selective Complexation of Alkali Metal Cations with Calix[4]Crowns in Aqueous Media: A Density Functional Theory Study" S. A. Baker, B. Ramachandran, and P. Derosa, oral presentation at the Louisiana Academy of Sciences annual meeting, Hammond, LA, February 27, 2009.
- “Cyclopropanation reactions of halomethylithium carbenoids: A computational study,” B. Ramachandran and L. M. Pratt, at the Southern School of Computational Chemistry, Jackson State University, June 29, 2009.
- “Computational Strategies for Reactions of Aggregated and Solvated Organolithium Carbenoids,” B. Ramachandran, Purnima Kharidehal, and L.M. Pratt, at the 2010 Mardi-Gras Conference on Computational Materials Science and Methods, Louisiana State University, February 11-14, 2010.
- “Computational Strategies for Reactions of Aggregated and Solvated Organolithium Carbenoids,” B. Ramachandran, Purnima Kharidehal, and Lawrence M. Pratt, at the Southern School of Computational Chemistry, Jackson State University, April 23-24, 2010.

SERVICE

A. College/University Service (Last five years; highlights only)

- Campus Computing Services Coordinating Committee (1992-present).

- Program Chair of Chemistry (1996-1998).
- Chemistry Faculty Search Teams each year since 1997, except for 1999-00 when there were no Chemistry positions advertised. Chaired the team in 1997-98 as Program Chair.
- 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)

B. Professional Service

- Scientific publication referee for the following journals (ongoing)
 - Chemical Physics Letters*,
 - J. Mol. Struct. (THEOCHEM)*,
 - Computer Physics Communications*,
 - Proceedings of the Louisiana Academy of Sciences*,
 - Journal of Physical Chemistry A*
 - Journal of Physical Chemistry B*
 - Journal of Chemical Physics*
 - Journal of the American Chemical Society*
 - Journal of Computational Chemistry*
- Proposal referee for the following funding organizations (ongoing)
 - American Chemical Society* (Petroleum Research Fund).
 - National Science Foundation* (Theoretical and Computational Chemistry Division).
- Software reviewer for *The Journal of Chemical Education* (1993-94).
- Session Chair for the session on “Excited State Dynamics and Photophysics,” at the Gordon Research Conference on Atomic and Molecular Interactions, New London, NH, June 1998.
- Session chair at the Eighth Conference on Current Trends in Computational Chemistry, at Vicksburg, MS, Nov. 5-6, 1999.
- Louisiana Optical Network Initiative (LONI) Resource Allocation Committee (2006-present)
- Louisiana Optical Network Initiative (LONI) Software Committee (2006-present)

- Southern Universities Research Association (SURA) JSA Programs (Jefferson Lab) Committee (2008-present)
- Organized “Conference on Molecular Structure and Dynamics” (24 speakers, ~100 attendees) to honor Professor Robert E. Wyatt, January 8-10, 2009, Austin, TX.
- Organized “Mardi Gras 2010 Conference on Computational Materials and Methods” (28 speakers, 80 attendees), February 11-14, 2010, Baton Rouge, LA.

REFERENCES

Available upon request.