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RESEARCH EXPERIENCE

Rensselaer Polytechnic Institute, Troy, NY, 1999-2002, 2004-present
Bioinformatics group, Wadsworth Center, Albany, NY, 2003
Marquette University, Milwaukee, 1998
University of Bonn, Bonn, Germany: Alexander von Humboldt Fellow 1993-95, 1997
Indian Institute of Technology, Madras, India: Pool Officer 1992-93
Panjab University, Chandigarh, India: Research Associate 1988-90, Visiting Fellow 1990-91
University of New Orleans, New Orleans: Research Associate 1985-87
University of Southern California, Los Angeles: Research Associate 1984-85

Current Research and Achievements

The Rensselaer Exploratory Center for Cheminformatics Research
<http://reccr.chem.rpi.edu/>

The Automated Design and Discovery of Novel Pharmaceuticals using Semi-Supervised Learning in Large Molecular Databases <http://www.drugmining.com/>

Electronic characterization and prediction of DNA transcription factor binding sites
[DIXEL](#)

Design and development of the [RECON](#) software package for rapid atomic-fragment-based molecular descriptor generation.

EDUCATIONAL QUALIFICATIONS

Ph.D. Chemistry, State University Of New York, Stony Brook, 1984
M.Sc. Chemistry, Indian Institute Of Technology, Kanpur, 1979 - First Division, Distinction
B.Sc.(Hons.Chemistry) St.Xavier's College, University of Calcutta, India, 1976

Computer Skills

Extensive programming experience in Fortran, Java, C++, PERL, HTML, Basic

Worked on IBM, Digital, Sun, HP, Apollo, Silicon Graphics and Cray platforms in Unix, Windows, Linux, VMS, MSDOS and X-Windows environments.

Experience with Gaussian, Jaguar, Spartan, Sybyl, MOE, Macromodel and other computational chemistry packages.

Experience with statistical modeling techniques, such as PCA, PLS, genetic algorithms, neural networks.

MANAGEMENT EXPERIENCE

Commercial Software Development and Consultancy and managing my own private business enterprise (Theorie International, Madras, India 1992-97)

Editorial - with Indian Science Association, Calcutta, India 1973-79

TEACHING EXPERIENCE

Theorie International, Madras, India 1992-93,95-97 (computer education)

Panjab University, Chandigarh, India - Visiting Fellow 1990-91 (General Chemistry, Molecular Reaction Dynamics)

State University of New York, Stony Brook, 1979-84 (Teaching Assistant for General Chemistry, Physical Chemistry, Molecular Structure and Spectroscopy Lab.)

Indian Science Association School for Scientific Education, Calcutta, India, 1976 (general science education)

AWARDS AND HONOURS

Alexander von Humboldt Foundation Fellowship 1993-95, 1997

Young Scientist Scheme, Department of Science and Technology, Govt. of India, 1990

Distinction in M.Sc. program, Indian Institute of Technology, Kanpur, India 1979

PROFESSIONAL MEMBERSHIPS

American Physical Society (life)

American Chemical Society

American Association for the Advancement of Science

Indian Science Association (President and Board of Advisors 1972-82)

Indian Association of College-Going Scientists (Ex-Officio 1976-79)

Schenectady Photographic Society (President 2003-2004)

LANGUAGES

English, Hindi, Sanskrit, Tamil, Bengali, German (Zertifikat Deutsch als Fremdsprache)

PUBLICATION HIGHLIGHTS

- Authored 34 research articles in refereed physics, chemistry, biology and philosophy journals, including 6 scientific book chapters
- Presented research papers at 45 national and international conferences

- Photo publication credits in national magazine and conference photo presentation
- Invited lectures in USA, India, Germany, Switzerland, Italy, Sweden, France
- Authored several popular science articles
- Authored and developed software packages for filing scientific literature, for financial accounting, for the electronic characterization and prediction of DNA transcription factor binding sites ([DIXEL](#)) and for rapid atomic-fragment-based molecular descriptor generation for virtual high throughput screening and drug design ([RECON](#))

BOOK CHAPTERS

1. N. Sukumar and Curt M. Breneman, "QTAIM in Drug Discovery and Protein Modeling" in "The Quantum Theory of Atoms in Molecules: From Solid State to DNA and Drug Design" C.F. Matta & R.J. Boyd, Eds. (Wiley-VCH, 2007)
2. C. Matthew Sundling, N. Sukumar, Hongmei Zhang, Curt M. Breneman and Mark J. Embrechts, "Wavelets in Chemistry and Cheminformatics" in Reviews in Computational Chemistry, Vol. 22, Kenny B. Lipkowitz, Thomas R. Cundari and Valerie J. Gillet (Eds), Wiley-VCH, Hoboken, pp. 295-329 (2006)
3. Curt M. Breneman, Minghu Song, Jinbo Bi, N. Sukumar, Kristin P. Bennett, Steven Cramer and Nihal Tugcu, "Prediction of Protein Retention Times in Anion-exchange Chromatography Systems using Support Vector Regression" in Chemometrics and Chemoinformatics, ACS Symp. Ser. 894, Barry K. Lavine (Ed.), American Chemical Society, pp. 111-125 (2005)
4. Curt M. Breneman and N. Sukumar, "New Developments in Molecular Modeling" in "Yearbook of Science & Technology" (McGraw-Hill, New York, 2004)
5. Curt M. Breneman, Kristin P. Bennett, Mark Embrechts, Steven Cramer, Minghu Song, Jinbo Bi and N. Sukumar, "Descriptor Generation, Selection and Model Building in Quantitative Structure-Property Analysis" in "Experimental Design for Combinatorial and High Throughput Materials Development" James N. Cawse, Ed. (John Wiley, New York, 2002), pp.203-238
6. N. Sukumar "Cellular Automaton Simulation of Solitonic Structures in the Su-Schrieffer-Heeger Hamiltonian" in "New Challenges in Comp. Quantum Chem." R.Broer, P.J.C.Aerts and P.S.Bagus, Eds., Univ.Groningen, The Netherlands, pp. 270-277 (1993)

RESEARCH PUBLICATIONS

(in refereed international journals)

1. C. Bergeron, T. Hepburn, M. Sundling, N. Sukumar, W. P. Katt, K. P. Bennett, C. M. Breneman, "Prediction of peptide bonding affinity: Kernel methods for nonlinear modeling" Protein Peptide Lett, in press, 2008.
2. N. Sukumar, "The Chemist's Concept of Molecular Structure" *Foundations of Chemistry*, in press, 2008.
3. N. Sukumar, Michael Krein and Curt M. Breneman, "Bio- and Chem-Informatics: Where do the twain meet?" *Curr. Opinion Drug Disc. Devel.* 11(3) 311-319 (May 2008)

4. Changjian Huang, Mark J. Embrechts, N. Sukumar and Curt M. Breneman, "Data Fusion and Auto-fusion for Quantitative Structure-Activity Relationship (QSAR)" Lecture Notes in Computer Science, 4668/2007, p.628-637 (Springer, Berlin / Heidelberg, 2007)
5. Scott Oloff, Shuxing Zhang, Nagamani Sukumar, Curt Breneman and Alexander Tropsha, "Chemometric Analysis of Ligand Receptor Complementarity: Identifying Complementary Ligands Based on Receptor Information (CoLiBRI)" *J. Chem. Inf. Model.* **46** (2), 844 – 851 (2006)
6. Minghu Song, Curt M. Breneman and N. Sukumar, "Three-Dimensional Quantitative Structure-Activity Relationship Analyses of Piperidine-based CCR5 Receptor Antagonists" *Bioorg. Med. Chem.* **12**, 489-499 (2004)
7. Curt M. Breneman, C. Matthew Sundling, N. Sukumar, Lingling Shen, William P. Katt and Mark J. Embrechts, "New developments in PEST shape/property hybrid descriptors" *J. Computer-Aided Mol. Design*, **17**, 231–240, (2003)
8. Christopher E. Whitehead, Curt M. Breneman, N. Sukumar and M. D. Ryan, "Transferable Atom Equivalent Multi-Centered Multipole Expansion Method" *J. Comp. Chem.* **24**, 512-529 (2003)
9. N. Tugcu, M.H. Song, C.M. Breneman, N. Sukumar, K.P. Bennett, and S.M. Cramer, "Prediction of the effect of mobile-phase salt type on protein retention and selectivity in anion exchange systems" *Analytical Chemistry*, **75**, 3563-3572 (2003)
10. Minghu Song, Curt M. Breneman, Jinbo Bi, N. Sukumar, Kristin P. Bennett, Steven Cramer and Nihal Tugcu, "Prediction of Protein Retention Times in Anion-exchange Chromatography Systems using Support Vector Regression" *J. Chem. Inf. Comput. Sci.* **42**, 1347-1357 (2002)
11. Cecilia B. Mazza, N. Sukumar, Curt M. Breneman and Steven Cramer, "Prediction of Protein Retention in Ion-Exchange Systems Using Molecular Descriptors Obtained from Crystal Structure" *Analytical Chemistry*, **73**, 5457-5461 (2001)
12. Chutian Shu, N. Sukumar and C. P. Ursenbach, "Adsorption of O₂ on TiO₂(110): A theoretical study" *J. Chem. Phys.* **110**, 10539-10544 (1999)
13. N. Sukumar and S. D. Peyerimhoff, "Nonadiabatic coupling of the 1A' and 2A' states of Ozone in the vicinity of their conical intersection and construction of Diabatic States" *Mol. Phys.* **95**, 61-70 (1998)
14. P. Raveendran, N. Sukumar and T. K. K. Srinivasan, "Temperature Dependence of Phonon-Assisted Luminescence Intensity in GdTb(MoO₄)₃ Evidence for change in Electron-Lattice Coupling near T_c", *Phys. Rev.* **B 55**, 4978-4982 (1997)
15. Harjinder Singh, N. Sukumar and B. M. Deb, "Atom as a Complex System: One- and Two-Dimensional Cellular Automata Simulations", *Int. J. Quantum Chem.* **60**, 21-28 (1996)
16. Thomas Neuheuser, N. Sukumar and S. D. Peyerimhoff, "Nonadiabatic Coupling of the ¹A" and ²A" States of Ozone", *Chem. Phys.* **194**, 45-64 (1995)
17. N. Sukumar "Density Functional Theory of Born Couplings", *Int. J. Quantum Chem.* **56**, 423-432 (1995)
18. N. Sukumar "Density Functional Theory for Jahn-Teller Systems", *Int. J. Quantum Chem.* **52**, 809-816 (1994)

19. N. Sukumar "Cellular Automaton Simulation of Solitonic Structures in the Su-Schrieffer-Heeger Hamiltonian" in "New Challenges in Comp. Quantum Chem.", R. Broer, P.J.C. Aerts and P.S. Bagus, Eds., Univ. Groningen, The Netherlands, pp. 270-277 (1993)
20. N. Sukumar "Comment on 'Electron Flow and Electronegativity Equalization in the process of bond formation'" J. Chem. Phys. **100**, 5390 (1994)
21. N. Sukumar, Harjinder Singh and B. M. Deb, "Electron Charge and Current Densities, the Geometric Phase and Cellular Automata", Z. Naturforschung **48a**, 134-136 (1993)
22. B. M. Deb, Ranbir Singh and N. Sukumar, "A Universal Density Criterion for Correlating the Radii and other Properties of Atoms and Ions" J. Molec. Struct. (Theochem) **259**, 121-139 (1992)
23. N. Sukumar and B. M. Deb, "Phase Associated with the Single-Particle Density of Many-Electron Systems" Intl. J. Quantum Chem. **40**, 501-510 (1991)
24. Jane S. Murray, Nagamani Sukumar, Shobha Ranganathan and Peter Politzer, "A Computational Analysis of the Electrostatic Potentials and Relative Bond Strengths of Hydrazine and some of its 1,1-Dimethyl Derivatives" Intl. J. Quantum Chem. **38**, 611-629 (1990)
25. Peter Politzer and Nagamani Sukumar, "An Examination of some Effects of OH Rotation in Phenol and p-Nitrophenol", J. Molec. Struct. (Theochem) **179**, 439-449 (1988)
26. Peter Politzer, Nagamani Sukumar, Keerthi Jayasuriya and Shoba Ranganathan, "Computational Evaluation and Comparison of some Nitramine Properties" J. Amer. Chem. Soc. **110**, 3425-3430 (1988)
27. Yongfeng Zhang, Nagamani Sukumar, Jerry L. Whitten and Richard N. Porter, "Ab initio Evaluation of the Born Correction, Born Couplings and Higher Derivative Matrix Elements with Gaussian Lobe Orbitals", J. Chem. Phys. **88**, 7662-7670 (1988)
28. Nagamani Sukumar and Gerald A. Segal, "Effect of Aqueous Solvation upon the Electronic Excitation Spectrum of Glycine Zwitterion : A Theoretical CI Study" J. Amer. Chem. Soc. **108**, 6880-6884 (1986)

CONFERENCE PROCEEDINGS

- N. Sukumar "Born Couplings in H₃" American Physical Society March Meeting, Las Vegas 1986, Bull. Amer. Phys. Soc. **31**, 1083 (1986)
- N. Sukumar and R. N. Porter "Breakdown of the Born-Oppenheimer approximation in a Jahn-Teller System : Calculation of the Born Coupling terms in H₃" SouthWest Theoretical Chemistry Conference, Rice University, Houston, 1986
- N. Sukumar "Importance of Electrostatic Considerations in the Study of Intermolecular Interactions" American Physical Society Spring Meeting, Crystal City, VA 1987, Bull. Amer. Phys. Soc. **32**, 1085 (1987)
- N. Sukumar "Investigation of the Polarization of Molecules in an Inhomogeneous Electron Gas Model" 1987 American Conference on Theoretical Chemistry, Gull Lake, MN, J. Phys. Chem. (microfiche suppl. 1987)

- N. Sukumar “Gauge Fields, Fibre Bundles and Diagrams for Radiationless Nonadiabatic Processes” Indian Academy of Sciences Discussion Meeting on Trends in Theoretical Chemistry, Indian Institute of Technology, Madras, 1990, Proc. Ind. Acad. Sci. (Chem. Sci.) 1992
- N. Sukumar “A ‘Radiative’ Theory for Radiationless Nonadiabatic Phenomena” University of Madras Seminar on Photochemistry, Laser Chemistry and Photobiology: Fundamentals and Applications, 1991
- N. Sukumar, Harjinder Singh and B. M. Deb, “One-Dimensional Toy Models for the Electron Densities in Disordered Systems using Stochastic Cellular Automaton Rules”, Proceedings of the International Conference on Disordered Materials (Structure and Properties) Ed. S.K. Srivastava, D. A. University, Indore, India, 1991
- N. Sukumar and D. Magesh, “Cellular Automaton Simulation of a Quasi-1-D Polymer”, One-Day Symposium on Mathematical Methods and Applications, Indian Institute Of Technology, Madras, 1992
- N. Sukumar, “Cellular Automata in Computational Quantum Chemistry”, First European Conference on Computational Chemistry, Nancy, France, 1994
- N. Sukumar, “On the Radii of Atoms and Ions” 5th WATOC, Jerusalem, 1996
- T. V. Gopalkrishnan and N. Sukumar, “The Symmetry of Music and its Cognition in the Human Brain”, Conference on Vedic Sciences, Chennai, India, 1997
- N. Sukumar, “Effect of Boundary Conditions on Cellular Automata that Classify Density”, Los Alamos eprint archive, 1998, <http://xxx.lanl.gov/abs/comp-gas/9804001>
- Curt M. Breneman, Nagamani Sukumar, Kristin P. Bennett, Mark J. Embrechts, Matthew Sundling and Larry Lockwood, “Wavelet representations of molecular electronic properties: Applications in ADME, QSPR and QSAR”, 220th National Meeting of the American Chemical Society, Washington, DC, Aug.2000
- N. Sukumar, Curt M. Breneman, Cecilia B. Mazza and Steven Cramer, “Predicting biomolecular recognition phenomena using the TAE/RECON method”, 220th National Meeting of the American Chemical Society, Washington, DC, Aug.2000
- N. Sukumar, C. Breneman, K. Bennett, M. Embrechts, M. Sundling and L. Lockwood, “TAE/RECON method in large database mining, QSAR, and ADME: A progress report on the DDASSL project”, *Pacificchem 2000 - fourth International Chemical Congress of Pacific Basin Societies, Honolulu, Hawaii, December 2000*
- M. Embrechts, C. Breneman, K. Bennett, Nagamani Sukumar, “GA approaches for successful QSAR modeling”, *Pacificchem 2000 - fourth International Chemical Congress of Pacific Basin Societies, Honolulu, Hawaii, December 2000*
- N. Sukumar, C. M. Breneman, and W. P. Katt, “Virtual high-throughput screening of large datasets using TAE/RECON descriptors”, 221st National Meeting American Chemical Society, San Diego, April 2001
- C. M. Breneman, K. P. Bennett, M. J. Embrechts, J. Bi, A. Demiriz, L. Lockwood Jr., M. Momma, and N. Sukumar, “Boosting support vector machines for VHTS, ADME and QSAR”, 221st National Meeting American Chemical Society, San Diego, April 2001

- Minghu Song, N. Sukumar, Asif Ladiwala, Jinbo Bi, Larry Lockwood, Steven Cramer and Curt M. Breneman. "Recent Development of RECON/TAE Method for Prediction of Protein Retention in Ion-Exchange Systems", Biotechnology in the Capital Region conference: Imaging and Bioengineering, Rensselaerville, New York, September 2001
- Minghu Song, Wei Deng, Matthew Sundling, N. Sukumar, Asif Ladiwala, Steven Cramer and Curt M. Breneman, "Displacer Efficiency Prediction by Electronic Shape/Property-Encode Descriptors", Biotechnology in the Capital Region conference: Imaging and Bioengineering, Rensselaerville, New York, September 2001
- Qiong Luo, N. Sukumar and Curt M. Breneman, "Features of Conformation-Sensitive TAE Descriptors for Protein Modeling", Biotechnology in the Capital Region conference: Imaging and Bioengineering, Rensselaerville, New York, September 2001
- Curt M. Breneman, N. Sukumar, Steven Cramer, Minghu Song, Asif Ladiwala, Mark Embrechts and Kristin Bennett, "Virtual High-Throughput Screening of Molecular Properties using Transferable Atom Equivalent (TAE) Techniques", A.I.Ch.E. National Meeting, Reno, Nevada, Nov.2001
- N. Sukumar, Curt M. Breneman, Dechuan Zhuang, William P Katt, Mark J Embrechts and Kristin Bennett, "The use of RECON/PEST software and electron density-derived descriptors for virtual high throughput database screening and refinement", 223rd National Meeting American Chemical Society, Orlando, April 2002
- N. Sukumar, Curt M. Breneman, C. Matthew Sundling, Lingling Shen, Minghu Song, Qiong Luo, Bo Jiang, Bill Katt and Hongmei Zhang, "New developments in PEST shape/property hybrid descriptors", 224th National Meeting American Chemical Society, Boston, August 2002
- N. Sukumar, Charles E. Lawrence, Curt M. Breneman, Kristin P. Bennett and Inna Vitol, "Fuzzy bar code representations of DNA-protein interactions", 226th National Meeting American Chemical Society, New York, September 2003
- N. Sukumar, Charles E. Lawrence, Curt M. Breneman, Kristin P. Bennett and Inna Vitol, "Dixel modeling of gene expression", 227th National Meeting American Chemical Society, Anaheim, March 2004
- N. Sukumar, "Phase and Gauge Transformations and Evolution of the Chemist's Concept of Molecular Structure", *International Society for the Philosophy of Chemistry, 2005 Summer Symposium*, Nashville, August 2005
- N. Sukumar, Curt M. Breneman, Steven M. Cramer, Kristin P. Bennett, Matthew Sundling, Qiong Luo and Dechuan Zhuang, "Intelligent Data Mining for Modeling and Prediction of Protein-Protein Protein-Surface and Protein-DNA Interactions", *Pacificchem 2005 - International Chemical Congress of Pacific Basin Societies, Honolulu, Hawaii*, December 2005
- N. Sukumar, Curt M. Breneman, Steven M. Cramer, James A. Moore, Kristin P. Bennett, Mark J. Embrechts, Min Li, Jia Liu and Long Han, "Closing the Loop: From High-throughput Screening to Synthesis of Novel Protein Displacers", *231st National Meeting American Chemical Society*, Atlanta, March 2006

POPULAR SCIENCE ARTICLES

Regular contributor to the Indian Science Association Newsletter, 1972-1980

PHOTO PUBLICATION CREDITS

- PSA journal – cover and photo-essay “*Slot canyons of the Colorado plateau*” (Photographic Society of America, June 2002)
- HART magazine, Issue # 7 (Newburgh Center for the Arts, N.Y., Nov.1999)
- FOCUS, Schenectady Photographic Society, Summer 2007, March 2008

INVITED LECTURES

- Hindustan Lever Research Centre, Bombay, India, 1987
- Second Winter School on Molecular Dynamics, Indian Institute Of Technology, Kanpur, 1988
- IDL Nitro-Nobel Basic Research Institute, Bangalore, India, 1988
- Department of Inorganic and Physical Chemistry, Indian Institute of Science, Bangalore, 1988
- School of Physical Sciences, Jawaharlal Nehru University, Delhi, 1988
- Department of Physical Chemistry, Indian Association for the Cultivation of Science, Jadavpur, Calcutta, 1988
- Discussion Meeting on Electronic Structure, Indian Institute of Science, Bangalore, 1989
- Bergische University Gesamthochschule Wuppertal, Germany, 1991
- Institute for Theoretical Chemistry, University of Bonn, Germany, 1991
- Laboratory for chemical and mineralogical Crystallography, University of Bern, Switzerland, 1991
- Institute of Quantum Chemistry, Uppsala University, Sweden, 1991
- Indian Academy of Sciences Discussion Meeting on Trends in Theoretical Chemistry, Indian Institute Of Technology, Kharagpur, 1993
- Workshop on Density Matrices, Sagamore XI Conference on Charge, Spin and Momentum Densities, Brest, France, 1994
- Institute of Quantum Chemistry, Uppsala University, Sweden, 1994
- Institute for Mathematical Sciences, Madras, 1995, 2005
- Academy Discussion Meeting on Frontiers in Structural Chemistry, Indian Institute Of Technology, Madras, 1996
- Department of Physics, Marquette University, Milwaukee, 1998
- ICAGEN, Research Triangle Park, North Carolina, 2001
- Eastern New York Section, American Chemical Society, Albany, NY, 2008
- "Yatra Trails of the Indian Himalayas" Photographic Society of America International Conference of Photography, Portland, Oregon, 2008