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RESEARCH EXPERIENCE

- Shiv Nadar University, Dadri, India, 2012-present
- Rensselaer Polytechnic Institute, Troy, NY, 1999-2012 (Research Associate Professor 2006-12)
- Institute of Mathematical Sciences, Chennai, India, 2009-2010
- 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: Res. Assoc. 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

EDUCATIONAL QUALIFICATIONS

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

TEACHING EXPERIENCE

- Shiv Nadar University, Dadri, India 2012-present
- Theorie International, Madras (Chennai), India 1992-93, 1995-97
- Panjab University, Chandigarh, India - Visiting Fellow 1990-91
- State University of New York, Stony Brook, 1979-84
- Indian Science Association School for Scientific Education, Calcutta, India, 1976

ADMINISTRATIVE EXPERIENCE

- Head, Department of Chemistry, Shiv Nadar University, India, 2012-2016; Undergraduate Student Advisor and Convenor, Departmental Undergraduate Committee, 2016-present
- Chair, University Library Committee, Shiv Nadar University, India, 2013-present
- Director, Center for Informatics, Shiv Nadar University, India, 2012-present
- President, Schenectady Photographic Society, Schenectady, NY; 2003-2004; Slide Group Chair, 2001-2003, Fine Arts Chair, 2004-2012; Webmaster, 2004-2009; Editor, FOCUS, 2009-2012
- 2nd Vice Chair, Color Projected Imaging Division, Photographic Society of America, 2010-2012
- Secretary, Pallavi of the Capital District, Albany, NY, 2006-2009
- Indian Science Association, President and Board of Advisors 1972-82

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

- Associate of the Photographic Society of America, 2016
- Betty Barker Award, Schenectady Photographic Society, Schenectady, NY, 2005

COURSES TAUGHT

- Advanced Molecular Spectroscopy
- Art & Science of Color
- Chemical Binding
- Chemical Equilibrium
- Chemical Principles
- Computational Chemistry
- Drugs and Natural Remedies
- General Chemistry
- General Chemistry lab
- Informatics & Drug Discovery
- Molecular Reaction Dynamics
- Molecular Structure & Spectroscopy lab
- Molecules of Love, Lust & Passion
- Physical Chemistry
- Research Methodologies
- Scientific Epistemology & Consciousness

RESEARCH STUDENTS GUIDED

Mr. Ganesh Prabhu, Department of Chemistry, Shiv Nadar University, 2012-2017. Ph.D. thesis entitled "Diversity Oriented Synthesis of a Molecular Library, Analysis of Molecular Diversity through Network/Graph Measures and Correlation with Biological Activity Profile(s)" submitted Jan.2017

Mr. Pinaki Saha, Department of Chemistry, Shiv Nadar University, Ph.D. 2013-present.

Mr. S. Ganesh, Opportunities for Undergraduate Research, Shiv Nadar University, 2016.

MEMBERSHIPS

- American Physical Society (life)
- American Chemical Society (since 1998)
- American Association for the Advancement of Science (AAAS)
- Indian Science Association (President and Board of Advisors 1972-82)
- Indian Association of College-Going Scientists (Ex-Officio 1976-79)
- Schenectady Photographic Society (1999-2013)
- Photographic Society of America (since 2000), APSA

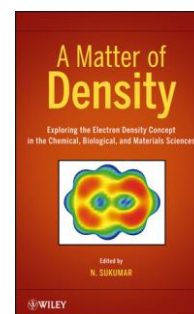
LANGUAGES

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

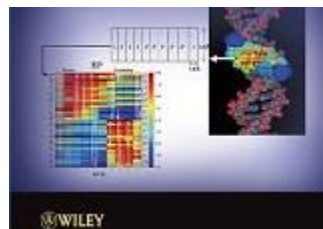
PUBLICATIONS

BOOKS & BOOK CHAPTERS

1. N. Sukumar, Ganesh Prabhu and Pinaki Saha, Applications of Genetic Algorithms in QSAR/QSPR modeling, Applications of Metaheuristics in Process Engineering, Eds: Jayaraman Valadi, Patrick Siarry (Springer, 2014) pp.315-324.
2. N. Sukumar, Ed. "A Matter of Density: Exploring the Electron Density Concept in Chemical, Biological, and Materials Sciences" (John Wiley, Hoboken, NJ, 2012). ISBN: 978-0-470-76900-3



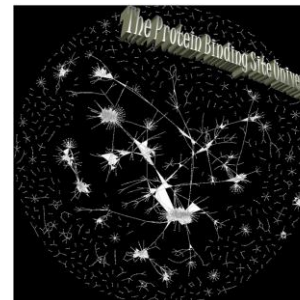
3. N. Sukumar, Michael P. Krein and Mark J. Embrechts, "*Predictive Cheminformatics in Drug Discovery: Statistical Modeling for Analysis of Micro-Array and Gene Expression Data*" in "Biocomputing and Drug Discovery" Richard S. Larson, Ed. (Humana Press, London, 2012).
4. N. Sukumar, Sourav Das, Michael Krein, Curt M. Breneman, Qiong Luo, Rahul Godawat, Shekhar Garde, Inna Vitol and Kristin P. Bennett, "*Molecular Descriptors for Biological Systems*" in "Computational Approaches in Cheminformatics and Bioinformatics" Rajarshi Guha and Andreas Bender, Eds. (John Wiley, Hoboken, NJ, 2012), pp.107-144.
5. N. Sukumar and Sourav Das, "Current trends in Virtual High-Throughput Screening using structure- and ligand-based methods" in "*Combinatorial Chemistry & High Throughput Screening*" B. Kundu, Ed. (Bentham) **14**, 872-888, 2011.
6. 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)
7. 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)
8. 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)
9. Curt M. Breneman and N. Sukumar, "*New Developments in Molecular Modeling*" in "Yearbook of Science & Technology" (McGraw-Hill, New York, 2004)
10. 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
11. 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 JOURNALS

12. Suman Kumar Mandal, Pinaki Saha, Parthapratim Munshi, N. Sukumar, Exploring Potent Ligand for Proteins: Insights from Knowledge-based Scoring Functions and Molecular Interaction Energies, *Struct. Chem.* **28**(5), 1537-1552 (2017). DOI: 10.1007/s11224-017-1007-y
13. Abdur Rahim, Pinaki Saha, Kunal Kumar, N. Sukumar, Bani Kanta Sarma, Reciprocal carbonyl–carbonyl interactions in small molecules and proteins, *Nature Comm.* **8**, 78 (2017). DOI: 10.1038/s41467-017-00081-x IF: 12.124
14. Pinaki Saha, Amol B. Rahane, Vijay Kumar, and N. Sukumar, Electronic Origin of the Stability of Transition Metal Doped B₁₄ Drum Shaped Boron Clusters and Their Assembly in to a Nanotube. *J. Phys. Chem. C*, **121**(20), 10728–10742 (2017). DOI: 10.1021/acs.jpcc.6b10838 IF: 4.536

15. Ke Wu, N. Sukumar, Nicholas A. Lanzillo, Chenchen Wang, Ramamurthy “Rampi” Ramprasad, Rui Ma, Aaron F. Baldwin, Greg Sotzing, Curt Breneman, Prediction of polymer properties using Infinite Chain Descriptors (ICD) and Machine Learning: Towards optimized dielectric polymeric materials, *J. Polymer Sci. B: Polymer Phys.* **54**, 2082–2091 (2016). DOI: 10.1002/polb.24117
16. Ganesh Prabhu, Sudepto Bhattacharya, Michael P. Krein, N. Sukumar, Investigation of similarity and diversity threshold networks generated from diversity-oriented and focused chemical libraries, *J. Math. Chem.* **54**(10), 1916-1941 (2016). DOI: 10.1007/s10910-016-0657-0 IF: 1.308
17. Pinaki Saha, Amol B. Rahane, Vijay Kumar, N. Sukumar, Analysis of the electron density features of small boron ring clusters and the effects of doping, *Physica Scripta* **91**, 053005 (2016). DOI: 10.1088/0031-8949/91/5/053005 IF: 1.126
18. N. Sukumar, M. P. Krein, G. Prabhu, S. Bhattacharya, S. Sen, Network Measures for Chemical Library Design, *Drug Development Research* **75**, 402–411 (2014) IF: 0.767
19. G. P. Pania, C. Wang, K. Wu, N. Sukumar, C. M. Breneman, G. A. Sotzing, R. Ramprasad, "New Group IV Chemical Motifs for Improved Dielectric Permittivity of Polyethylene" *J. Chem. Inf. Model.* **53**(4):879–886 (2013) DOI: 10.1021/ci400033h IF: 3.738
20. N. Sukumar, The atom in a molecule as a mereological construct in chemistry, *Found. Chem.* **15**(3), 303-309 (2013) DOI: 10.1007/s10698-012-9171-z IF: 1.361
21. N. Sukumar and Michael P. Krein, “Graphs and networks in chemical and biological informatics: past, present, and future” *Future Med. Chem.* **4** (16) (2012) DOI: 10.4155/fmc.12.128 IF: 3.744
22. N. Sukumar, Michael Krein, Qiong Luo and Curt Breneman, "MQSPR modeling in materials informatics: a way to shorten design cycles?" *J. Mater. Sci.*, **47**(21), 7703-7715 (2012). DOI: 10.1007/s10853-012-6639-0 (2012). IF: 2.371
23. Krein M. P., Sukumar N., Exploration of the Topology of Chemical Spaces with Network Measures. *J. Phys. Chem. A*, **115**(45), 12905-12918 (2011). DOI: 10.1021/jp204022u IF: 2.693
24. N. Sukumar, “The Chemist's Concept of Molecular Structure” *Found. Chem.*, **11** (1), 7-20 (2009) DOI: 10.1007/s10698-008-9060-7 IF: 1.361
25. Pankaj Kulshrestha, N. Sukumar, Jane S. Murray, Rossman F. Giese and Troy D. Wood, “Computational Prediction of Antibody Binding Sites on Tetracycline Antibiotics: Electrostatic Potentials and Average Local Ionization Energies on Molecular Surfaces” *J. Phys. Chem. A*, **113** (4), 756-766 (2009) DOI: 10.1021/jp8089165 IF: 2.693
26. 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) IF: 4.507
27. 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](http://arxiv.org/abs/1108.5397)" <http://arxiv.org/abs/1108.5397>
28. 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) IF: 0.51
29. Scott Oloff, Shuxing Zhang, N. 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) DOI: 10.1021/ci050065r IF: 3.738



30. 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) DOI: 10.1016/j.bmc.2003.10.019 IF: 2.793
31. 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) DOI: 10.1023/A:1025334310107 IF: 2.990
32. 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) DOI: 10.1002/jcc.10240 IF: 2.902
33. 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) DOI: 10.1021/ac0263519 IF: 5.636
34. 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) DOI: 10.1021/ci025580t IF: 2.902
35. 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" *Anal. Chem.*, **73**, 5457-5461 (2001) DOI:10.1021/ac010797s IF: 5.636
36. Chutian Shu, N. Sukumar and C. P. Ursenbach, "Adsorption of O₂ on TiO₂(110): A theoretical study" *J. Chem. Phys.* **110**, 10539-10544 (1999) DOI: 10.1063/1.478985 IF: 2.952
37. 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) IF: 1.720
38. 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) IF: 3.736
39. 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) IF: 1.432
40. Thomas Neuheuser, N. Sukumar and S. D. Peyerimhoff, "Nonadiabatic Coupling of the 1A' and 2A' States of Ozone", *Chem. Phys.* **194**, 45-64 (1995) IF: 1.652
41. N. Sukumar "Density Functional Theory of Born Couplings", *Int. J. Quantum Chem.* **56**, 423-432 (1995) IF: 1.432
42. N. Sukumar "Density Functional Theory for Jahn-Teller Systems", *Int. J. Quantum Chem.* **52**, 809-816 (1994) IF: 1.432
43. N. Sukumar "Comment on 'Electron Flow and Electronegativity Equalization in the process of bond formation'" *J. Chem. Phys.* **100**, 5390 (1994) IF: 2.952
44. 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) IF: 0.552
45. 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) IF: 1.545
46. N. Sukumar and B. M. Deb, "Phase Associated with the Single-Particle Density of Many-Electron Systems" *Int. J. Quantum Chem.* **40**, 501-510 (1991) IF: 1.432
47. Jane S. Murray, N. 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" *Int. J. Quantum Chem.* **38**, 611-629 (1990) IF: 1.432

48. Peter Politzer and N. Sukumar, "An Examination of some Effects of OH Rotation in Phenol and p-Nitrophenol", *J. Molec. Struct. (Theochem)* **179**, 439-449 (1988) IF: 1.545
49. Peter Politzer, N. Sukumar, Keerthi Jayasuriya and Shoba Ranganathan, "Computational Evaluation and Comparison of some Nitramine Properties" *J. Amer. Chem. Soc.* **110**, 3425-3430 (1988) IF: 12.113
50. Yongfeng Zhang, N. 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) IF: 2.952
51. N. 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) IF: 12.113

CONFERENCE PAPERS

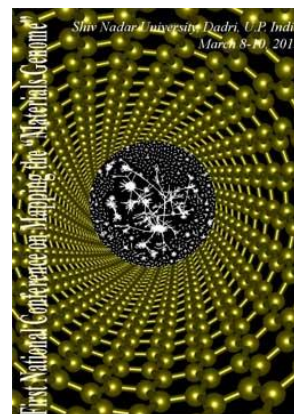
1. N. Sukumar "Born Couplings in H₃" *Amer. Phys. Soc. March Meet.*, Las Vegas 1986, *Bull. Amer. Phys. Soc.* **31**, 1083 (1986)
2. N. Sukumar and R. N. Porter "Breakdown of the Born-Oppenheimer approximation in a Jahn-Teller System: Calculation of the Born Coupling terms in H₃" *SW Theor. Chem. Conf.*, Rice University, Houston, 1986
3. N. Sukumar "Importance of Electrostatic Considerations in the Study of Intermolecular Interactions" *Amer. Phys. Soc. Spring Meet.*, Crystal City, VA 1987, *Bull. Amer. Phys. Soc.* **32**, 1085 (1987)
4. N. Sukumar "Investigation of the Polarization of Molecules in an Inhomogeneous Electron Gas Model" *1987 Amer. Conf. Theor. Chem.*, Gull Lake, MN, *J. Phys. Chem. (microfiche suppl. 1987)*
5. N. Sukumar "Gauge Fields, Fibre Bundles and Diagrams for Radiationless Nonadiabatic Processes" *Ind. Acad. Sci. Disc. Meet. Trends in Theor. Chem.*, Indian Institute of Technology, Madras, 1990, *Proc. Ind. Acad. Sci. (Chem. Sci.)* 1992
6. N. Sukumar "A 'Radiative' Theory for Radiationless Nonadiabatic Phenomena" *University of Madras Seminar on Photochemistry, Laser Chemistry and Photobiology: Fundamentals and Applications*, 1991
7. N. Sukumar, Harjinder Singh and B. M. Deb, "One-Dimensional Toy Models for the Electron Densities in Disordered Systems using Stochastic Cellular Automaton Rules", *Proc. Int. Conf. Disordered Materials (Structure and Properties)* Ed. S.K. Srivastava, D. A. University, Indore, India, 1991
8. N. Sukumar and D. Magesh, "Cellular Automaton Simulation of a Quasi-1-D Polymer", *One-Day Symp. Math. Methods and Applications*, Indian Institute of Technology, Madras, 1992
9. N. Sukumar, "Cellular Automata in Computational Quantum Chemistry", *First European Conf. Comput. Chem.*, Nancy, France, 1994
10. N. Sukumar, "On the Radii of Atoms and Ions" 5th WATOC, Jerusalem, 1996
11. T. V. Gopalkrishnan and N. Sukumar, "The Symmetry of Music and its Cognition in the Human Brain", *Conf. on Vedic Sciences*, Chennai, India, 1997
12. 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>
13. Curt M. Breneman, N. 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

14. N. Sukumar, Curt M. Breneman, Cecilia B. Mazza and Steven Cramer, "Predicting biomolecular recognition phenomena using the TAE/RECON method", *220th Nat. Meet. Amer. Chem. Soc.*, Washington, DC, Aug.2000
15. 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 Int. Chem. Cong. Pacific Basin Soc.*, Honolulu, Hawaii, December 2000
16. M. Embrechts, C. Breneman, K. Bennett, N. Sukumar, "GA approaches for successful QSAR modeling", *Pacificchem 2000 - fourth Int. Chem. Cong. Pacific Basin Soc.*, Honolulu, Hawaii, December 2000
17. N. Sukumar, C. M. Breneman, and W. P. Katt, "Virtual high-throughput screening of large datasets using TAE/RECON descriptors", *221st Nat. Meet. Amer. Chem. Soc.*, San Diego, April 2001
18. 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 Nat. Meet. Amer. Chem. Soc.*, San Diego, April 2001
19. Minghu Song, Curt M. Breneman, Jinbo Bi, Muhsin Ozdemir, N. Sukumar, Mark J. Embrechts, and Kristin Bennett, "GA-PLS, SVM and NN modeling of CACO-2 permeability using TAE descriptors", *COMP 222nd Nat. Meet. Amer. Chem. Soc.*, Chicago, August 2001
20. 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
21. 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
22. 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
23. 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", *AICChE. Nat. Meet.*, Reno, Nevada, Nov.2001
24. 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 Nat. Meet. Amer. Chem. Soc.*, Orlando, April 2002
25. 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 Nat. Meet. Amer. Chem. Soc.*, Boston, August 2002
26. 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
27. N. Sukumar, Charles E. Lawrence, Curt M. Breneman, Kristin P. Bennett and Inna Vitol, "Dixel modeling of gene expression", *227th Nat. Meet. Amer. Chem. Soc.*, Anaheim, March 2004
28. Qiong Luo, Asif Ladiwala, Dechuan Zhuang, N Sukumar, Curt M Breneman Steve M. Cramer, "Development of protein moment descriptors and pH-dependent descriptors for

- prediction of protein affinity in hydrophobic interaction chromatography systems”, *228th Nat. Meet. Amer. Chem. Soc.*, Philadelphia, August 2004
29. N. Sukumar, Curt M. Breneman and Mark J. Embrechts, “Electron density derived descriptors in ADME/Tox screening”, *229th Nat. Meet. Amer. Chem. Soc.*, San Diego, March 2005
 30. N. Sukumar, “Phase and Gauge Transformations and Evolution of the Chemist’s Concept of Molecular Structure”, *Int. Soc. Phil. Chem., 2005 Summer Symp.*, Nashville, August 2005
 31. 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 – Int. Chem. Cong. Pacific Basin Soc., Honolulu, Hawaii*, December 2005
 32. 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 Nat. Meet. Amer. Chem. Soc.*, Atlanta, March 2006
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 34. N. Sukumar, Curt M. Breneman and C. Matthew Sundling, “New tools for virtual high-throughput screening”, *232nd Nat. Meet. Amer. Chem. Soc.*, San Francisco, September 2006
 35. Jia Liu, Min Li, N. Sukumar, Curt M. Breneman and Steven M. Cramer, “Identification of novel chemically selective displacers from commercial chemical databases using an SVM classification model and parallel batch screening experiments”, *232nd Nat. Meet. Amer. Chem. Soc.*, San Francisco, September 2006
 36. N. Sukumar, Curt M. Breneman, Kristin P. Bennett, Charles Bergeron, Theresa Hepburn, C. Matthew Sundling, Shekhar Garde, Rahul Godawat, Ishita Manjrekar, Margaret McLellan and Mike Krein, “Bio- and chem-Informatics: Where do the twain meet?”, *234th Nat. Meet. Amer. Chem. Soc.*, Boston, August 2007
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 38. Jed Zaretski, Curt M. Breneman, Charles Bergeron, N. Sukumar and Mike Krein, “A reactivity and recognition component-based methodology for computational prediction of likely sites of CYP 450 3A4-mediated metabolism”, *234th Nat. Meet. Amer. Chem. Soc.*, Boston, August 2007
 39. M. Dominic Ryan, Theresa Hepburn, N. Sukumar, Sourav Das and Curt M. Breneman, “TAE Augmented scoring functions: Two approaches, atom and surface based”, *234th Nat. Meet. Amer. Chem. Soc.*, Boston, August 2007
 40. Sourav Das, Curt M. Breneman, N. Sukumar and M. Dominic Ryan, “TAE augmented scoring functions: Application to enzymatic and nonenzymatic proteins”, *235th Nat. Meet. Amer. Chem. Soc.*, New Orleans, April 2008
 41. C. Matthew Sundling, Curt M. Breneman, Mark J. Embrechts, Changjian Huang, Xiaohua Wu and N. Sukumar, “Testing the limits of a QSAR model: How many cases are actually needed to develop a reliable predictive model?”, *235th Nat. Meet. Amer. Chem. Soc.*, New Orleans, April 2008
 42. Curt M. Breneman and N. Sukumar, “Cheminformatics developments at RECCR: New tools, collaborations and outreach”, *235th Nat. Meet. Amer. Chem. Soc.*, New Orleans, April 2008

43. Mark J. Embrechts, Curt M. Breneman, Changjian Huang and N. Sukumar, "Testing the validity range of QSAR models using one-class support vector machines", *235th Nat. Meet. Amer. Chem. Soc.*, New Orleans, April 2008
44. Sunanda Sukumar, Benjamin Woo, N. Sukumar, Arshad S. Kokardekar, Judith Klein-Seetharaman and Kalyan C. Tirupula, "Docking Studies of Dipeptides to Metabotropic Glutamate Receptors", *37th NE Reg. Meet. Amer. Chem. Soc.*, Burlington, VT, June 2008
45. Curt M. Breneman, N. Sukumar, Mike Krein, Margaret McLellan, Jed Zaretski, Sourav Das and Arshad Shirish Kokardekar, "How much computation is enough?", *236th Nat. Meet. Amer. Chem. Soc.*, Philadelphia, August 2008
46. L. C. Brinson, Linda S. Schadler, Curt M. Breneman, N. Sukumar, M. Kreim and R. Qiao, "Intelligent design of nanocomposites via informatics", *237th Nat. Meet. Amer. Chem. Soc.*, Salt Lake City, March 2009
47. N. Sukumar and Mike Krein, "Mapping the Network Topology of Chemical Spaces" *Central Regional Meeting of the American Chemical Society*, Cleveland, May 2009
48. N. Sukumar, Mike Krein and Curt M. Breneman, "Chemical space network topology through atom typing" *238th Nat. Meet. Amer. Chem. Soc.*, Washington, DC, August 2009
49. N. Sukumar, "Towards a mereology of structured wholes in chemistry and the sciences" *Int. Society Phil. Chem. Summer Symp.*, Philadelphia, August 2009
50. N. Sukumar, Michael P. Krein, "Mapping Chemical and Biological Networks using Molecular Fragments and Fingerprints" *CHI Structure-Based Drug Design conf.*, Cambridge, MA, June 2012
51. Ganesh Prabhu, Sudepto Bhattacharya, Michael Krein, N. Sukumar, "Network measures in polymer space" *First National Conference on Mapping the "Materials Genome"*, Shiv Nadar University, India, March 8-10, 2013
52. Swapnil Shukla, Kalpesh Shelke, Shameek Ghosh, Bimlesh Lochab, N. Sukumar, V. K. Jayaraman, "Modeling the Curing Characteristics of Monomers" *First National Conference on Mapping the "Materials Genome"*, Shiv Nadar University, India, March 8-10, 2013
53. N. Sukumar, Vijay Kumar, Electron density and bonding characteristics of structural isomers of (InN)₃₂ nanoparticles, *Gordon Research Conference on Electron Distribution & Chemical Bonding*, Les Diablerets, Switzerland, June 2-7, 2013.
54. N. Sukumar, Ganesh Prabhu, Sudepto Bhattacharya, Michael P. Krein, Subhabrata Sen, V. K. Jayaraman, Network Measures for Chemical Library Design, *Gordon Research Conference on Computer Aided Drug Design*, Mt. Snow, Vermont, USA, July 21 – 26, 2013.
55. N. Sukumar, Michael Krein, Ganesh Prabhu, Sudepto Bhattacharya, Subhabrata Sen, and V. K. Jayaraman, "Chemical Library Design using Graphical and Network measures" - *International Humboldt Kolleg on Bench to bedside translational research: Potential benefits of interdisciplinary collaboration*, Manipal, India, Nov.15-17, 2013.
56. N. Sukumar, M. P. Krein, G. Prabhu, S. Bhattacharya, S. Sen, "Network Measures for Chemical Library Design and Materials Informatics" - *XI Girona Seminar on Carbon, Metal, and Carbon-Metal Clusters: From Theory to Applications*, Girona, Spain, June 30-July 3, 2014.
57. N. Sukumar, K. Wu, P. Saha, C. M. Breneman, G. Pilania, C. C. Wang, G. Sotzing, R. Ramprasad, B. L. Chittari and V. Kumar, Materials informatics modeling for the design of advanced materials, *9th International Conference on Computational Physics (ICCP9)*, Singapore, January 7 – 11, 2015.

58. N. Sukumar, P. Saha, V. Kumar, A. Rahane, K. Wu, C. M. Breneman, Informatics modeling used to leverage first-principles computation for accelerated materials discovery, *Korean Physical Society*, April 22, 2015.
59. N. Sukumar, Pinaki Saha, Vijay Kumar, Amol B. Rahane, Analysis of the electron density features of boron clusters and effects of doping, *SAGAMORE XVIII Conference on Charge, Spin and Momentum Densities*, Santa Margherita di Pula, Sardinia, Italy, June 7-12, 2015.
60. N. Sukumar, Ganesh Prabhu, Sudepto Bhattacharya, Michael P.Krein, Disintegration of the small world property with increasing diversity of chemical libraries, *Gordon Research Conference on Computer Aided Drug Design*, Mt. Snow, West Dover, VT, USA, July 19-24, 2015.
61. Ganesh Prabhu, Subhabrata Sen, Sudepto Bhattacharya, Michael P.Krein, N. Sukumar, Quantifying the diversity of chemical libraries through network modeling, *250th Nat. Meet. Amer. Chem. Soc.*, Boston, MA, August 16–20, 2015.
62. Pinaki Saha, Amol B. Rahane, N. Sukumar, Vijay Kumar. Double ring tubular structures of boron clusters stabilized by metal atom doping: MB_{14} ($M = Cr, Fe, \text{ and } Ni$), *Intl. Symp. on Clusters, Cluster-Assemblies and Nanomaterials (ISCAN)*, Thiruvananthapuram, Kerala, March 9 - 12, 2016.
63. Pinaki Saha, Amol B. Rahane, Vijay Kumar, and N. Sukumar, Double ring tubular structures of boron clusters stabilized by metal atom doping: $M@B_{14}$ ($M = Cr, Fe, \text{ and } Ni$), *253rd Nat. Meet. Amer. Chem. Soc.*, San Francisco, CA, April 2-6, 2017.
64. Ganesh Prabhu, Vivek Ananth R.P., Jayaraman Valadi, Michael P.Krein, N. Sukumar, Descriptor Selection for QSAR Modelling using Network Measures, *Int. Conf, Drug Design*, April 7-9th, 2017.
65. Pinaki Saha, Amol B. Rahane, Vijay Kumar and N. Sukumar, $M@B_{14}$: A journey of a doped boron cluster from nanodrum to nanotube, Symposium on “Emerging Materials” Shiv Nadar University, 12 August 2017



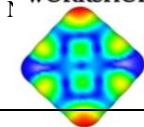
CONFERENCE ORGANIZATION

- Co-organizer, First National Conference on Mapping the “Materials Genome”, Shiv Nadar University, March 8-10, 2013
- Co-organizer, Workshop on Computational Nanoscience, Shiv Nadar University, March 30 – April 5, 2014
- Program advisory committee, One-day symposium on Emerging Trends in translational research in India, Shiv Nadar University, April 12, 2014
- Scientific Advisory Committee, International Conference on Green Initiatives in Science and Technology (GIST-2015), Manav Rachna College of Engineering, Faridabad, Jan. 15, 2015.
- Interdisciplinary Conference on the Science and Applications of Networks, Shiv Nadar University, March 20–22, 2015
- Scientific Advisory Committee, RSC Workshop on Chemistry for Tomorrow’s



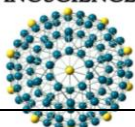
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30 MARCH - 5 APRIL 2014

Hosted by the Centre of Informatics
School of Natural Sciences.



ORCID 0000-0002-2724-9944

World, New Delhi, December 2-3, 2015.

EDUCATION

N. Sukumar, "Cross-disciplinary Education for Fostering Critical Thinking", E-QUAL News, 4(1), 5-7, January 2017

PHOTOGRAPHY BOOKS/ARTICLES

- N. Sukumar, "Slot canyon photography", *Photographic Society of America Journal*, June 2002
- N. Sukumar, "Essence" (Blurb, Inc. 2009)
- N. Sukumar, "Integration" (Blurb, Inc. 2011)



PHOTOGRAPHY CONFERENCE PRESENTATIONS & AWARDS

- "Double Vision" Schenectady Photographic Society Photo Essay of the Year 2006-2007
- "Iona" Schenectady Photographic Society Digital Projected Image of the Year 2007-2008
- "Yatra Trails of the Indian Himalayas" Photographic Society of America International Conference of Photography, Portland, Oregon, Sept. 2008.
- "Double Vision" Community Zoe festival, 29 Palms, California, 2008
- "Essence" Schenectady Photographic Society Print Photo Essay of the Year 2008-2009
- "Sandstone Symphony: The American Southwest – A World of Abstracts" 9th International Conference, Photographic Association of Dum Dum, Kolkatta, India, Jan. 2010
- "Patterns of India" Schenectady Photographic Society Photo Essay of the Year 2010-2011
- "Rock Dance" Schenectady Photographic Society Projected Image of the Year 2011
- "Sandstone Symphony: Abstracts of the American Southwest" Photographic Society of America International Conference of Photography Colorado Springs, Sept. 2011.
- "Sandstone Symphony" FestX 2011, Todos Santos, Baja California, Mexico, Oct. 2011.
- "Integration" - 10th International Conference on Photography, Photographic Association of Dum Dum, Kolkatta, India, Jan.23-27, 2014.
- Elected Associate (APSA) of the Photographic Society of America (awarded Sept. 2016)
- N, Sukumar & Sunanda Sukumar "Using Photography to Integrate the Teaching of Humanities, Arts and Sciences" - 11th International Conference on Photography, Photographic Association of Dum Dum, Kolkatta, India, Jan.23-27, 2017.

SOLO & JURIED EXHIBITIONS

- Solo Exhibit, Exhibited at *Art Finds*, Colonie, NY, Nov.1999-April 2000
- Solo Exhibit, Exhibited at Zuzu's, Albany, April-June 2000
- Albany Photoregional, Albany, NY, 2000
- Fulton Street Gallery, Troy, NY, 2002
- Art Space Gallery, Norwich, CT, 2003
- Fulton Street Gallery, Troy, NY, 2004
- Albany Photoregional, Albany, NY, 2005
- Fulton Street Gallery, Troy, NY, 2005-6
- Albany Photoregional, Albany, NY, 2007
- Photography Center of the Capital District, Troy, NY, 2007

- Fulton Street Gallery, Troy, NY, 2008
- Photography Center of the Capital District, Troy, NY, 2008
- Photography Center of the Capital District, Troy, NY, 2009
- *New Visions*, The Center for Fine Art Photography, Fort Collins, CO, 2010
- Solo Exhibit, Mc Greevy Pro Lab, Albany, Aug.-Sept. 2010
- Arts & Architecture, Ottawa, Canada, 2011

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 of Mathematical Sciences, Madras, 1995.
- 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.
- Institute of Mathematical Sciences, Chennai, India, 2005.
- Eastern New York Section, American Chemical Society, Albany, NY, 2008.
- Department of Chemistry and Institute of Theoretical Sciences, Indian Institute of Technology, Kharagpur, India, Dec. 2009.
- “*Some mathematical problems from Cheminformatics*” Institute of Mathematical Sciences, Chennai, India, Jan. 2010.
- “*The Elephant and the Flea: Cheminformatics (& Bioinformatics) with electron density derived descriptors*” Indian Institute of Science Education and Research, Mohali, India, Feb. 2010.
- “*Cheminformatics and Bioinformatics: Electron Density to Network Topology*” Indian Institute of Science, Bangalore, Jan. 7, 2011
- Central Drug Research Institute Diamond Jubilee Lecture, Lucknow, India, Jan. 12, 2011.
- “*Predictive Cheminformatics, Bioinformatics and Virtual High Throughput Screening: Statistical Modeling for Analysis of Micro-Array and Gene Expression Data*” National Training on Bioinformatics in multi-Omics Era: A Microbial Genomics Perspective, National Bureau of Agriculturally Important Microorganisms Maunath Bhanjan, UP, Feb. 28, 2012.

- “*Network thinking in Chemistry and Biology*” - Keynote address - National Conference on Emergence of Interdisciplinary Sciences, Jodhpur, Aug. 25, 2012.
- National Training on Bioinformatics: Computational Tools for Microbial Research, at National Bureau of Agriculturally Important Microorganisms, Maunath Bhanjan, UP, Nov.19-30, 2013.
- “*Chemical properties derived from the electron density and its critical points*”, Workshop on Computational Nanoscience, Shiv Nadar University, March 30 –April 5, 2014.
- “*Cheminformatics and Statistical Modeling in Materials and Life Sciences*”, Workshop on electronic structure, atomistic and statistical modeling in Chemistry, Materials and Life Sciences, University of Delhi, October 8-10, 2014.
- “*Materials design through ab initio computations and statistical modeling*”, Korea Advanced Institute of Science and Technology (KAIST), Daejeon, South Korea, April 22, 2015.

REVIEWER for:

Austrian Academy of Sciences, Doctoral Fellowship Programme
 Combinatorial Chemistry & High Throughput Screening
 Computational and Theoretical Chemistry
 Current Computer-Aided Drug Design
 Current Medicinal Chemistry
 Foundations of Chemistry
 Future Medicinal Chemistry
 Gene Regulation and Systems Biology
 IEEE Transactions on Nanotechnology
 Journal of Chemical Information and Modeling
 Journal of Chemical Physics
 Journal of Chemical Sciences
 Journal of Materials Science
 Journal of Medicinal Chemistry
 Journal of Molecular Structure: THEOCHEM
 Journal of Receptor, Ligand and Channel Research
 Journal of the Royal Society Interface
 Medicinal Chemistry
 Mini-Reviews in Medicinal Chemistry
 Molecular Informatics
 Molecules
 Physics Letters A
 Polymer Engineering and Science
 Science & Engineering Research Board, India
 Wellcome Trust/ DBT India Alliance