Complete list of research publications (including research papers, contributed chapters and books) of Shridhar R. Gadre

1. The role of starting voltage in the kinetics of decomposition of ammonia under electric discharge	T. S. Rao S. R. Gadre H. A. Patil	Z. Naturforsch. **28a**, 803 (1973)
2. Calculation of atomic and molecular energies from experimental Compton profiles	S. R. Gadre P. T. Narasimhan	Mol. Phys. **31**, 1613 (1976)
3. Empirical correlation between energy and Compton profile in isoelectronic series	S. R. Gadre P. T. Narasimhan	Nat. Acad. Sci. Letters (India) **1**, 21 (1977)
4. Single and double Gaussian FSGO model and Compton profiles	S. R. Gadre P. T. Narasimhan	Chem. Phys. Letters **50**, 247 (1977)
5. Electron momentum distributions from valence-bond wave functions	S. R. Gadre P. T. Narasimhan	Intern. J. Quantum Chem. **12**, 105 (1977)
6. Electron momentum distributions and Compton profiles from FSGO wave functions	S. R. Gadre R. Ramaswamy P. T. Narasimhan	Pramana **8**, 99 (1977)
7. Compton profiles of free-and crystal-ions from Hartree-Fock and Hartree-Fock-Slater wave functions	S. R. Gadre P. T. Narasimhan	Intern. J. Quantum Chem. **12 (S1)**, 173 (1977)
8. Some inequalities among expectation values of one-electron operators in atomic system.	S. R. Gadre	J. Chem. Phys. **71**, 1510 (1979)
9. Local density functional theory of atoms and molecules	R. G. Parr S. R. Gadre L. J. Bartolotti	Proc. Nat. Acad. Sci. (U.S.A.) **76**, 2522 (1979)
10. An application of information theory to Compton profiles	S. R. Gadre S. B. Sears	J. Chem. Phys. **71**, 4321 (1979)
11. On the basic homogeneity characteristics of atomic and molecular energies	R. G. Parr S. R. Gadre	J. Chem. Phys. **72**, 3669 (1980)
12. Electronegativities of the element from simple X-alpha theory	L. J. Bartolotti S. R. Gadre R.G. Parr	J. Amer. Chem. Soc. **102**, 2945 (1980)
13. Bounds for Coulomb energies	S. R. Gadre N. H. Handy L. J. Bartolotti	J. Chem. Phys. **72**, 1034 (1980)
14. Theoretical Compton profile anisotropies in molecules and solids - VIII. Vibrational and rotational dependence of Compton profiles	B. M. Pettitt S. R. Gadre R. L. Matcha	Intern. J. Quantum Chem. Symp. **14**, 697 (1980)

15. An information theoretic synthesis and analysis of Compton profiles	S. B. Sears S. R. Gadre	J. Chem. Phys. **75**, 4626 (1981)
16. Direct and reverse transformations between electron density and electron momentum density	S. R. Gadre R. K. Pathak	Phys. Rev. A**24**, 2906 (1981)
17. Estimation of <P> and <P^{-1}> from atomic electron densities	R. K. Pathak S. R. Gadre	J. Chem. Phys. **74**, 5925 (1981)
18. On representation of the Coulomb integral by one-electron functionals	S. R. Gadre R. K. Pathak	J. Chem. Phys. **75**, 4740 (1981)
19. Inequalities among atomic expectation values	S. R. Gadre R. L. Matcha	J. Chem. Phys. **74**, 589 (1981)
20. Novel DNA sequence organization in rice genome	V. Gupta S. R. Gadre P. K. Ranjekar	Biochem. Biophys. Acta **656**, 147 (1981)
21. On the monotonicity of atomic momentum densities and inequalities among atomic expectation values	S. R. Gadre R. L. Matcha	J. Chem. Phys. **76**, 748 (1982)
22. Estimation of <P> and <P^{-1}> from atomic densities : A comment	S. R. Gadre R. K. Pathak	J. Chem. Phys. **77**, 1073 (1982)
23. Electron momentum distributions and atomic <r^n >expection values	S. R. Gadre S. P. Gejji N. Venkatalaxmi	Phys. Rev. A**26**, 1768 (1982)
24. Local-density-functional model for atoms in momentum space	R. K. Pathak P. V. Panat S. R. Gadre	Phys. Rev. A**26**, 3073 (1982)
25. Lower bounds to the Weizsäcker correction	S. R. Gadre R. K. Pathak	Phys. Rev. A**25**, 668 (1982)
26. Relationships between the terms in the gradient expansion : Kinetic and exchange energy functionals	R. K. Pathak S. R. Gadre	Phys. Rev. A**25**, 3426 (1982)
27. On the monotonicity of the atomic electron momentum density and shell structure of the radial momentum density	S. R. Gadre R. K. Pathak S. Chakravorty	J. Chem. Phys. **78**, 4581 (1983)
28. Hartree-Fock momentum expectation values of atoms and ions	S. R. Gadre S. P. Gejji S. Chakravorty	At. Data Nucl. Data Tables **28**, 477 (1983).
29. Direct and reverse transformations between electron density and electron momentum density : Connection with the locally averaged method	S. R. Gadre S. P. Gejji R. K. Pathak	Phys. Rev. A**28**, 462 (1983)

30. Electron density to electron momentum density : The use of an energy constraint	S. R. Gadre S. P. Gejji R. K. Pathak	Phys. Rev. A**27**, 3328 (1983)
31. On representation of electron-electron repulsion energies by simple one-electron functionals	S. R. Gadre R. D. Bendale	J. Chem. Phys. **78**, 996 (1983)
32. Gradient-free representation of the Weizsäcker term for atoms	R. K. Pathak S. R. Gadre	Phys. Rev. A**28**, 1808 (1983)
33. Use of energy constraint for refinement of electron momentum distributions	S. R. Gadre S. P. Gejji	J. Chem. Phys. **80**, 175 (1984)
34. From molecular electron density to electron momentum density	R. K. Pathak S. P. Gejji S. R. Gadre	Phys. Rev. A**29**, 3402 (1984)
35. Extraction of molecular electron momentum densities from electron density contour maps	S. R. Gadre S. P. Gejji	Chem. Phys. Letters **112**, 45 (1984)
36. Information entropy and Thomas-Fermi theory	S. R. Gadre	Phys. Rev. A**30**, 620 (1984)
37. Refinement of electron momentum densities of ionic solids using an experimental energy constraint	S. R. Gadre S. P. Gejji	Chem. Phys. Letters **109**, 584 (1984)
38. Molecular analysis of cucurbitaceae genomes: II. Comparison of high resolution thermal denaturation profiles of DNA's in seven plant species	M. Bhave M. Lagu S. R. Gadre	Ind. J. Biochem. and Biophys. **21**, 81 (1984)
39. The self-interaction correction to the local spin density model : Effect on atomic momentum space properties	S. R. Gadre S. J. Chakravorty	Chem. Phys. Letters **120**, 101 (1985)

40. Analysis of atomic electron momentum densities : use of information entropies in coordinate and momentum space	S. R. Gadre R. D. Bendale S. P. Gejji	Chem. Phys. Letters **17**, 138 (1985)
41. Maximization of atomic information entropy sum in configuration and momentum spaces	S. R. Gadre R. D. Bendale	Intern. J. Quantum Chem. **28**, 311 (1985)
42. Information entropies in quantum chemistry	S. R. Gadre R. D. Bendale	Curr. Sci. (India) **54**, 970 (1985)
43. Some novel characteristics of atomic information entropies	S. R. Gadre S. B. Sears S. J. Chakravorty R. D. Bendale	Phys. Rev. A**32**, 2602 (1985)
44. A novel approach for the study of intermolecular interactions : molecular deformation densities	T. N. Guru Row S. R. Gadre	Proc. Ind. Acad. Sci. (Chem. Sci.) **95**, L437 (1985)
45. Electron density in chemistry	S. R. Gadre	Curr. Sci. **54**, 329 (1985)
46. Interconnections between atomic-electron density and electron-momentum density : Leading and tail correction	S. R. Gadre S. J. Chakravorty	Phys. Rev. A**33**, 1374 (1986)
47. Compton profiles of atoms from electron density via reciprocal from factors	S. R. Gadre S. J. Chakravorty	Proc. Ind. Acad. Sci. (Chem. Sci.) **96**, 241 (1986)
48. Some rigorous inequalities among the Weizsäcker correction, and atomic $<r^n>$ and $<p^n>$ values	S. R. Gadre S. J. Chakravorty	J. Chem. Phys. **84**, 7051 (1986)
49. The average electron momentum densities and rigorous bounds to average electron densities for atoms and molecules	S. R. Gadre S. J. Chakravorty	Chem. Phys. Letters **132**, 535 (1986)

50. On the similarity between molecular electron densities, electrostatic potentials and bare-nuclear potentials	S. R. Gadre R. D. Bendale	Chem. Phys. Letters **130**, 515 (1986)
51. Use of a nonlocal density approximation for the transformation from electron density to electron momentum density	S. R. Gadre S. J. Chakravorty	J. Chem. Phys. **86**, 2224 (1987)
52. Coulomb energy, total X-ray scattering intensities and average electron densities	S. J. Chakravorty S. R. Gadre	Chem. Phys. Letters **142**, 205 (1987)
53. Nonlocal-density approximation for exploring kinetic energy anisotropies	S. R. Gadre T. Koga S. J. Chakravorty	Phys. Rev. A**36**, 4155 (1987)
54. Rigorous relationships among quantum-mechanical kinetic energy and atomic information entropies : Upper and lower bounds	S. R. Gadre R. D. Bendale	Phys. Rev. A**36**, 1932 (1987)
55. Use of second-moment constraint for the refinement of determinantal wave function	S. R. Gadre S. A. Kulkarni I. H. Shrivastava	Phys. Rev. A**38**, 487 (1988)
56. Property-oriented basis-sets using cross-entropy minimzation	S. R. Gadre S. A. Kulkarni I. H. Shrivastava	Portugalea Fisica **19**, 349 (1988)
57. Bounds to electron-repulsion energies	S. R. Gadre R. K. Pathak	Proc. Ind. Acad. Sci. (Chem. Sci.) **100**, 483 (1988)
58. Development of links between electron densities in complementary spaces	R. K. Pathak S. R. Gadre	Portugalea Fisica **19**, 407 (1988)
59. Rigorous bounds to molecular electron repulsion and electrostatic potential integrals	S. R. Gadre S. A. Kulkarni R. K. Pathak	J. Chem. Phys. **91**, 3596 (1989)

60. Reduced first-order density matrices and "exchange-only" correlation factors for closed-shell atomic systems	S. R. Gadre S. A. Kulkarni R. K. Pathak	Phys. Rev. A**40**, 4224 (1989)
61. Interconnections between electron densities in position and momentum spaces	S. R. Gadre R. K. Pathak	A Chapter in a book: **Aspects of many body effects in molecules and extended systems**, Ed. D. Mukherjee, Lecture notes in Chem. Vol. **50**, Springer (1989)
62. Atomic and molecular diamagnetic susceptibilities from Compton scattering data	S. R. Gadre R. K. Pathak	J. Chem. Phys. **92**, 4327 (1990)
63. Momentum space atomic first-order density matrices and "exchange-only" correlation factors	R. K. Pathak S. A. Kulkarni S. R. Gadre	Phys. Rev. A**42,** 2622 (1990)
64. Cross-entropy minimization for refinement of Gaussian basis-sets*	S. R. Gadre S. A. Kulkarni I. H. Shrivastava	Chem. Phys. Letters **166,** 445 (1990)
65. Applications of rigorous bounds for efficient evaluation of molecular electrostatic potentials	S. R. Gadre I. H. Shrivastava S. A. Kulkarni	Chem. Phys. Letters **170**, 271 (1990)
66. Nonexistence of local maxima in molecular electrostatic potential maps	S. R. Gadre R. K. Pathak	Proc. Ind. Acad. Sci. (Chem. Sci.) **102**, 189 (1990)
67. Maximal and minimal characteristics of molecular electrostatic potentials	R. K. Pathak S. R. Gadre	J. Chem. Phys. **93**, 1770 (1990)
68. A general parallel algorithm for the generation of molecular electrostatic potential maps	S. R. Gadre S. V. Bapat K. Sundararajan I. H. Shrivastava	Chem. Phys. Letters **175**, 307 (1990)

69. Some investigations on symmetry and external properties of molecular electron momentum densities	S. R. Gadre A. C. Limaye S. A. Kulkarni	J. Chem. Phys. **94**, 8040 (1991)
70. Computation of molecular electrostatic potential : An efficient algorithm and parallelization	S. R. Gadre S. Bapat I. H. Shrivastava	Comp. and Chem. **15**, 203 (1991)
71. Reply to the comment on: Maximal and minimal characteristics of molecular electrostatic potentials: Some further extensions	S. R. Gadre S. A. Kulkarni R. K. Pathak	J. Chem. Phys. **94**, 8639 (1991)
72. Some aspects of parallelization of two-electron integrals in molecular orbital programs	S. R. Gadre S. A. Kulkarni A. C. Limaye R. N. Shirsat	Zeit. Phys. - D : Atoms, Molecules and Clusters **18**, 357 (1991)
73. Shapes and sizes of molecular anions via topographical analysis of electrostatic potential	S. R. Gadre I. H. Shrivastava	J. Chem. Phys. **94**, 4384 (1991)
74. Parallelization of two electron integrals in molecular orbital programs	S. R. Gadre S. A. Kulkarni A. C. Limaye A. Taspa	A Chapter in ***Advanced Computing***, Ed. V. P. Bhatkar, Tata Mc Graw Hill (1991), p. 388-391
75. Algorithm development and parallelization of molecular electrostatic potential	S. R Gadre S. Bapat I. H. Shrivastava	A Chapter in ***Advanced Computing***, Ed. V. P. Bhatkar, Tata Mc Graw Hill (1991), p. 388-391
76. Bounds to atomic and molecular energy functionals	S. R. Gadre R. K. Pathak	Adv. Quantum Chem. **22**, 211, Ed. P.-O. Löwdin, Academic, New York (1991)
77. Molecular electrostatic potentials: A topographical study	S. R. Gadre S. A. Kulkarni I. H. Shrivastava	J. Chem. Phys. **96**, 5253 (1992)

78. Deriving chemical parameters from electrostatic potential maps of molecular anions	S. R. Gadre C. Kölmel I. H. Shrivastava	Inorg. Chem. **31**, 2279 (1992)
79. Topographical view of molecular electron-momentum densities	S. A. Kulkarni S. R. Gadre R. K. Pathak	Phys. Rev. A**45**, 4399 (1992)
80. Molecular electrostatics of $[V_{10}O_{28}]^{6-}$ cluster : a graphics visualization study using PARAM	S. R. Gadre S. Bapat A. Taspa R. N. Shirsat	Curr. Sci. (India) **62**, 798 (1992)
81. Molecular electrostatics. A comprehensive topographical approach	R. N. Shirsat S. V. Bapat S. R. Gadre	Chem. Phys. Letters **200**, 373 (1992)
82. Development of a restricted Hartree-Fock program INDMOL on PARAM: A highly parallel computer	R. N. Shirsat A. C. Limaye S. R. Gadre	J. Comput. Chem. **14**, 445 (1993)
83. Density-based electron localization function via nonlocal density approximation	S. R. Gadre S. A. Kulkarni R. K. Pathak	J. Chem. Phys. **98**, 3574 (1993)
84. Visualization of shapes of molecular anions	S. R. Gadre C. Kölmel M. Ehrig R. Ahlrichs	Z. Naturforsch. -A **48**, 137 (1993)
85. On the topography of electron momentum densities of linear molecules	S. A. Kulkarni S. R. Gadre	Z. Naturforsch. -A **48**, 145 (1993)
86. Momentum space investigation of C_{2v} dissociation of water	S. R. Gadre S. A. Kulkarni	Proc. Ind. Acad. Sci. (Chem. Sci.) **105**, 149 (1993)
87. Topography-driven electrostatic charge models for molecules	S. R. Gadre I. H. Shrivastava	Chem. Phys. Letters **204**, 350 (1993)
88. Probing chemical reactions in momentum space	S. A. Kulkarni S. R. Gadre	J. Amer. Chem. Soc. **115**, 7434 (1993)

89. Radii of monopositive atomic ions	S. R. Gadre K. D. Sen	J. Chem. Phys. **99**, 3149 (1993)
90. SCRF calculation of the effect of hydrogen on the topology of molecular electrostatic potential	F. J. Luque M. Orozco P. K. Bhadane S. R. Gadre	J. Phys. Chem. **97**, 9380 (1993)
91. Molecular electrostatic charge models: a topographical approach	I. H. Shrivastava S. R. Gadre	Intern. J. Quantum Chem. **49**, 397 (1994)
92. Graphics visualization of molecular surfaces	S. R. Gadre A. Taspa	J. Mol. Graphics **12**, 45 (1994)
93. Electrophilic additions to 7-methylenenorbornenes and 7-isopropylidenenobornenes: Can remote substituents swamp electrostatic control of □-face selectivity?	G. Mehta G. Gunasekaran S. R. Gadre R. N. Shirsat B. Ganguly J. Chandrasekhar	J. Org. Chem. **59**, 1953 (1994)
94. Electrostatic vs. Orbital control of facial selectivities in π systems: Experimental and theoretical study of electrophilic additions to 7-isoprpylidenenobornanes**	G. Mehta F. A. Khan S. R. Gadre R. N. Shirsat B. Ganguly J. Chandrasekhar	Angew. Chem. Int. Ed. Engl. **33**, 1390 (1994)
95. A general parallel solution to the integral transformation and second-order Møller-plesset evaluation on distributed memory parallel machines	A. C. Limaye S. R. Gadre	J. Chem. Phys. **100**, 1303 (1994)
96. Comment on "Computing molecular electrostatic potentials with PRISM algorithm"	S. R. Gadre R. N. Shirsat	Chem. Phys. Letters **218**, 593 (1994)

97. Effect of solvation on the shapes, sizes and anisotropies of polyatomic anions via molecular electrostatic potential topology: An *ab initio* self-consistent reaction field approach	F. J. Luque M. Orozco P. K. Bhadane S. R. Gadre	J. Chem. Phys. **100**, 6718 (1994)
98. Bonding and delocalization in C_{60} via topographical analysis of the electrostatic potential and electron density	T. A. Claxton R. N. Shirsat S. R. Gadre	J. Chem. Soc. Chem. Commun. **731** (1994)
99. A "critical" appraisal of electrostatic charge models for molecules	S. R. Gadre S. S. Pundlik I. H. Shrivastava	Proc. Ind. Acad. Sci. (Chem. Sci.) **106**, 303 (1994)
100. Molecular tailoring approach for simulation of electrostatic properties	S. R. Gadre R. N. Shirsat A. C. Limaye	J. Phys. Chem. **98**, 9165 (1994)
101. Closo-boranes, -carboranes, and silaboranes: A topographical study using electron density and molecular electrostatic potential	E. D. Jemmis G. Subramanian I. H. Shrivastava S. R. Gadre	J. Phys. Chem. **98**, 6445 (1994)
102. The effect of hydration on the molecular charge distribution of cations. An *ab initio* SCRF study	F. J. Luque S. R. Gadre P. K. Bhadane M. Orozco	Chem. Phys. Letters **232**, 509 (1995)
103. Basis set dependence of the molecular electrostatic potential topography. A case study of substituted benzenes	S. R. Gadre S. A. Kulkarni C. H. Suresh I. H. Shrivastava	Chem. Phys. Letters **239**, 273 (1995)
104. An *ab initio* topographical investigation on the electrostatic potential of some chemical mutagens	A. K. Bhattacharya S. S. Pundlik S. R. Gadre	Curr. Sci. (India) **69**, 58 (1995)
105. Topographical analysis of electron density and molecular electrostatic potential for cyclopropa- and cyclobutabenzenes	S. R. Gadre S. S. Pundlik	J. Amer. Chem. Soc. **117**, 9559 (1995)

106. Structure, energetics and bonding of diacetylene complexes with hydrogen fluoride. A theoretical investigation	A. K. Chandra S. Pal A. C. Limaye S. R. Gadre	Chem. Phys. Letters **247**, 95 (1995)
107. Electron localization in molecules: a comparative study of scalar fields	S. A. Kulkarni S. R. Gadre	J. Mol. Struct. (THEOCHEM) **361**, 83 (1996)
108. An electrostatic investigation: how polar are ionic surfactant hydrocarbon tails?	S. R. Gadre S. S. Pingale	Chem. Commun. **595** (1996)
109. Steric enhancement of resonance: An electron localization perspective	S. R. Gadre L. J. Bartolotti C. H. Suresh	Curr. Sci. (India) **71**, 130 (1996)
110. Molecular recognition via electrostatic potential topography	S. R. Gadre P. K. Bhadane S. S. Pundlik S. S. Pingale	Molecular electrostatic potential: concepts and applications, chapter 5, Ed. J. Murray and K. D. Sen, Elsevier, Amsterdam (1996), p. 219-522
111. Personal computer based visualization of three dimensional scalar and vector fields: an application to molecular graphics	A. C. Limaye P. V. Inamdar S. M. Dattawadkar S. R. Gadre	J. Mol. Graphics **14**, 19 (1996)
112. Molecular electrostatic potential topographical studies on the structural motifs of C_{60}	E. D. Jemmis G. Subramanian G. N. Sastry G. Mehta R. N. Shirsat S. R. Gadre	J. Chem. Soc. Perkin Trans. **2**, 2343 (1996)
113. Electronic perturbations of the aromatic nucleus: Hammett constants and electrostatic potential topography	S. R. Gadre C. H. Suresh	J. Org. Chem. **62**, 2625 (1997)

114. Complementary electrostatics for the study of DNA base pair interactions	S. R. Gadre S. S. Pundlik	J. Phys. Chem. B **101**, 3298 (1997)
115. Electrostatic potential as a harbinger of cation coordination: $CF_3SO_3^-$ ion as a model example	S. P. Gejji L. J. Bartolotti C. H. Suresh S. R. Gadre	J. Phys. Chem. B **101**, 5678 (1997)
116. How reliable are topographical characteristics of Hartree-Fock level molecular electron momentum densities?	S. A. Kulkarni S. R. Gadre	Chem. Phys. Letters **274**, 255 (1997)
117. Structure and stability of DNA base trimers: An electrostatic approach	S. S. Pundlik S. R. Gadre	J. Phys. Chem. B **101**, 9657 (1997)
118. Patterns in hydrogen bonding via electrostatic potential topography	S. R. Gadre P. K. Bhadane	J. Chem. Phys. **107**, 5625 (1997)
119. Conformational and electrostatic properties of naphthazarin, juglone and naphthaquinone: an *ab initio* theoretical study	A. K. Bhattacharya S. S. Pundlik S. R. Gadre	Cancer Investigation **15**, 531 (1997)
120. Electrostatic investigation of metal cation binding to DNA bases and base pairs	S. S. Pundlik S. R. Gadre A. C. Limaye A. P. Rendell	Chem. Commun. 573 (1998)
121. A novel electrostatic approach to substituent constants: Doubly substituted benzenes	C. H. Suresh S. R. Gadre	J. Amer. Chem. Soc. **120**, 7049 (1998)
122. Face selectivity in electrophilic additions to methylenenoranoutanes: relative importance of through-space, through-bond and electrostatic interactions	G. Mehta C. Ravikrishna S. R. Gadre C. H. Suresh P. Kalyanaraman J. Chandrasekhar	Chem. Commun. 975 (1998)

123. Theoretical studies on the structures of $M^+BF_4^-$ ion pairs (M= Li, NH_4): the role of electrostatics and electron correlation	C. H. Suresh S. R. Gadre S. P. Gejji	Theor. Chem. Acc. **99**, 151 (1998)
124. Polarization-corrected electrostatic potential for probing cation binding patterns of molecules. 1. Saturated hydrocarbons	S. R. Gadre S. S. Pingale	J. Amer. Chem. Soc. **120**, 7056 (1998)
125. Complexes of ammonia with propane and cyclopropane: electrostatic guidelines for *ab initio* treatment	S. R. Gadre P. K. Bhadane	Theor. Chem. Acc. **100**, 300 (1998)
126. Co-operative electrostatics for understanding crown ether hydration patterns	S. R. Gadre S. S. Pingale	Curr. Sci. (India) **75**, 1162 (1998)
127. Electrostatic insights into molecular hydration process: A case study of crown ethers	S. S. Pingale S. R. Gadre L. J. Bartolotti	J. Phys. Chem. A**102**, 9987 (1998)
128. Clar's aromatic sextet theory revisited via molecular electrostatic potential topography	C. H. Suresh S. R. Gadre	J. Org. Chem. **64**, 2505 (1999)
129. Molecular electrostatics for exploring complexes of carbonyl compounds with hydrogen fluoride	S. R. Gadre P. K. Bhadane	J. Phys. Chem. A**103**, 3512 (1999)
130. Electrostatics in chemistry. 1 Basic principles	S. R. Gadre P. K. Bhadane	Resonance **4 (2)**, 8 (1999)
131. Electrostatics in chemistry. 2 electrostatic potentials of atoms, ions and molecules	S. R. Gadre P. K. Bhadane	Resonance **4 (5)**, 40 (1999)

132. Electrostatics in chemistry. 3 molecular electrostatic potential: visualization and topography	S. R. Gadre P. K. Bhadane	Resonance **4 (7)**, 14 (1999)
133. Electrostatics in chemistry. 4 electrostatics models for weak molecular complexation	S. R. Gadre K. Babu	Resonance **4 (12)**, 11 (1999)
134. *Ab initio* structure and vibrational frequencies of $(CF_3SO_2)_2\bar{N}Li^+$ ion pairs	S. P. Gejji C. H. Suresh K. Babu S. R. Gadre	J. Phys. Chem. A**103**, 7474 (1999)
135. Topography of atomic and molecular scalar fields	S. R. Gadre	An invited article in **Computational Chemistry: Reviews in Current Trends**, Vol. **4,** Ed. J. Leszczynski, World Scientific, Singapore (1999), p. 1-53
136. Molecular electrostatics for exploring hydration patterns of molecules: 2. Formamide	S. R. Gadre A. D. Kulkarni	Special issue on contemporary theoretical chemistry research in India, Ind. J. Chem. A**39**, 50 (2000)
137. Molecular electrostatic potential and electron density topography: Structure and reactivity of (substituted arene) $Cr(CO_3)$ complexes	C. H. Suresh N. Koga S. R. Gadre	Organometallics **19**, 3008 (2000)
138. Electrostatics for exploring hydration patterns of molecules: 3. Uracil	S. R. Gadre K. Babu A. P. Rendell	J. Phys. Chem. A **104**, 8976 (2000)

139. Does a stacked DNA base pair hydrate better than a hydrogen-bonded one? : An *ab initio* study	D. Sivanesan K. Babu S. R. Gadre V. Subramanian T. Ramasami	J. Phys. Chem. A **104**, 10887 (2000)
140. Electrostatics of atoms and molecules	S. R. Gadre R. N. Shirsat	An educational monograph published by Universities Press, Hyderabad (2000)
141. Univis-2000: An indigenously developed comprehensive visualization package	A. C. Limaye S. R. Gadre	Curr. Sci. (India) **80**, 1296 (2001)
142. Polarization-corrected molecular electrostatic potential for the cation binding problem	S. R. Gadre S. S. Pingale	Chem. Phys. Lett. **340**, 604 (2001)
143. Theoretical investigation on structure, electrostatic potentials and vibrational frequencies of diglyme and Li^+(diglyme) conformers	S. P. Gejji S. R. Gadre V. J. Barge	Chem. Phys. Lett. **344**, 527 (2001)
144. Revisiting Markovnikov addition to alkenes via molecular electrostatic potential	C. H. Suresh N. Koga S. R. Gadre	J. Org. Chem. **66**, 6883 (2001)
145. Structure and stability of water clusters $(H_2O)_n$, n= 8–20: An *ab initio* investigation	S. Maheshwary N. Patel N. Sathyamurthy A. D. Kulkarni S. R. Gadre	J. Phys. Chem. A **105**, 10525 (2001)
146. H-π complexes of acetylene-ethylene: A matrix isolation and computational Study	K. Sundararajan K. Sankaran K. S. Viswanathan A. D. Kulkarni S. R. Gadre	J. Phys. Chem. A **106,** 1504 (2002)

147. H…□ complexes of acetylene-benzene: a matrix isolation & computational study	K. Sundarajan K. S. Viswanathan A. D. Kulkarni S. R. Gadre	J. Mol. Str. **613**, 209 (2002)
148. Exciplex emission from the mixed dimer of naphthalene & 2-cyanonphthalene in a supersonic jet	A. Das K. K. Mahato C. K. Nandi T. Chakraborty S. R. Gadre N. A. Gokhale	Phys. Chem. Chem. Phys. **4**, 2162 (2002)
149. Electrophilic additions to a 2-methylenebicyclo [2.1.1] hexane system: Probing π-face selectivity for electrostatic and orbital effects	G. Mehta S. R. Singh P. Balanarayan S. R. Gadre	Org. Lett. **4,** 2297 (2002)
150. *Ab initio* quality one-electron properties of large molecules: Development and testing of molecular tailoring approach	K. Babu S. R. Gadre	J. Comput. Chem. **24,** 484 (2003)
151. Information theoretical approaches to quantum chemistry	S. R. Gadre	A chapter in **Reviews of Modern Quantum Chemistry :** **A Celebration of the Contributions of Robert G. Parr**, Vol. **1,** Ed. K. D. Sen, World Scientific, Singapore (2003), p. 108-147
152. Topography of molecular scalar fields. I. Algorithm and Poincaré–Hopf relation	P. Balanarayan S. R. Gadre	J. Chem. Phys. **119,** 5037 (2003)
153. Electrostatics-guided *ab initio* studies on weakly bonded complexes of substituted naphthalenes	S. R. Gadre M. M. Deshmukh T. Chakraborty	Chem. Phys. Lett. **384,** 350 (2004)

154. Exploring hydration patterns of aldehydes and amides : *Ab initio* investigations	A. D. Kulkarni K. Babu S. R. Gadre L. J. Bartolotti	J. Phys. Chem. A **108**, 2492 (2004)
155. Tailoring approach for exploring electron densities and electrostatic potentials of molecular crystals	K. Babu V. Ganesh S. R. Gadre N. E. Ghermani	Theor. Chem. Acc. **111**, 255 (2004) An invited article in a special issue honoring Professor Jacopo Tomasi
156. Many-body interaction analysis: Algorithm development and applications to large molecular clusters	A. D. Kulkarni V. Ganesh S. R. Gadre	J. Chem. Phys. **121**, 5043 (2004)
157. Structure, reactivity and aromaticity of acenes and their BN analogs : A density functional and electrostatic investigation	A. K. Phukan R. P. Kalagi S. R. Gadre E. D. Jemmis	Inorg. Chem. **43**, 5824 (2004)
158. Molecular interpretation of water structuring and destructuring effect : Hydration of alkanediols	M. M. Deshmukh N. V. Sastry S. R. Gadre	J. Chem. Phys. **121**, 12402 (2004)
159. Quantum chemical investigations on explicit molecular hydration	S. R. Gadre M. M. Deshmukh R. P. Kalagi	Proc. Ind. Nat. Sci. Acad. Professor P. T. Narasimhan festschrift Thematic Issue **70** A**,** 709 (2004)
160. Is there a hydrogen bond radius? Evidence from microwave spectroscopy, neutron scattering and x-ray diffraction results.	B. Lakshmi A. G. Samuelson K. V. Jovan Jose S. R. Gadre E. Arunan	New J. Chem. **2**, 371 (2005)
161. Topography of molecular scalar fields. II. An appraisal of the hierarchy principle for electron momentum densities	P. Balanarayan S. R. Gadre	J. Chem. Phys. **122**, 164108 (2005)

162. Molecular tailoring approach for *ab initio* treatment of large molecules	S. R. Gadre K. Babu V. Ganesh	A chapter in **Recent Trends in Practice and Theory of Information Technology: Proceedings of NRB Seminar**, Editor S. N. Maheshwari, Viva Books, New Delhi (2005), p. 86
163. Adsorption of water on sodium chloride surfaces: Electrostatics-guided *ab initio* studies	A. Pramanik R. P. Kalagi V. J. Barge S. R. Gadre	Theor. Chem. Accts. **114**, 129 (2005), Invited article in Special Issue honoring Professor Karl Jug
164. Why are carborane acids so acidic? An electrostatic interpretation of Brønsted acid strengths	P. Balanarayan S. R. Gadre	Inorg. Chem. **44**, 9613 (2005)
165. Molecular electrostatic potential (MESP) studies on the anti-hyperglycemic agents – 2,5-digydroxyquinones	D. S. Patel P. Daga P. V. Bharatam R. K. Dongare S. R. Gadre	Indian J. Chem. Sec A **45**, 13 (2006)
166. Atoms-in-molecules in momentum space: A Hirshfeld partitioning of electron momentum densities	P. Balanarayan S. R. Gadre	J. Chem. Phys. **124**, 204113 (2006)
167. Can ring strain be realized in momentum Space?	P. Balanarayan S. R. Gadre	J. Amer. Chem. Soc. **128,** 10702 (2006)
168. Molecular tailoring approach for geometry optimization of large molecules: energy evaluation and parallelization strategies	V. Ganesh R. K. Dongare P. Balanarayan S. R. Gadre	J. Chem. Phys. **125,** 104109 (2006)
169. Estimation of intramolecular hydrogen bonding via molecular tailoring approach	M. M. Deshmukh S. R. Gadre L. J. Bartolotti	J. Phys. Chem. A **110**, 12519 (2006)
170. Molecular tailoring approach : Towards PC-based *ab initio* treatment of large molecules	S. R. Gadre V. Ganesh	J. Theor. Comp. Chem. **5**, 835 (2006)
171. Electrostatic potential minimum of the aromatic ring as a measure of substituent constant	C. H. Suresh S. R. Gadre	J. Phys. Chem. A **111**, 710 (2007)

172. Electrostatic potential topography for exploring electronic reorganizations in 1, 3 dipolar cycloadditions	P. Balanarayan R. Kavathekar S. R. Gadre	J. Phys. Chem. A **111**, 2733 (2007)
173. Intramolecular hydrogen bond Energy In Polyhydroxy Systems: A critical comparison of molecular Tailoring and Isodesmic reaction Approaches	M. M. Deshmukh C. H. Suresh S. R. Gadre	J. Phys. Chem. A **111**, 6472 (2007)
174. *Ab initio* treatment of Large Molecules : Cut-and-Stitch the Tailor's Way	S. R. Gadre A. P. Rahalkar V. Ganesh	Indian Assoc. Nucl. Chem. Allied Sci. V, 267 (2007)
175. Effect of matrix on IR frequencies of acetylene and acetylene-methanol complex: Infrared matrix isolation and *ab initio* study	K. V. Jovan Jose S. R. Gadre K. Sundararajan K. S. Viswanathan	J. Chem. Phys. **127**, 104501 (2007)
176. Is corannulene a better diene or dienophile? A DFT analysis	P. Jayapal M. Sundararajan G. Rajaraman P. Venuvanalingam R. Kalagi S. R. Gadre	J. Phys. Org. Chem. **21**, 146 (2008)
177. Intermolecular hydrogen bonding and cooperative interactions in carbohydrates via the molecular tailoring approach	M. M. Deshmukh L. J. Bartolotti S. R. Gadre	J. Phys. Chem. A **112**, 312 (2008)
178. Web Prop: Web Interface for *Ab Initio* calculation of molecular one-electron properties	V. Ganesh R. Kavathekar A. P. Rahalkar S. R. Gadre	J. Comp. Chem. **29**, 488 (2008)
179. An *ab initio* investigation on (CO_2)n and (CO_2)n Ar_m clusters: Geometries and IR spectra	K. V. Jovan Jose S. R. Gadre	J. Chem. Phys. **128**, 124310 (2008)
180. Quantum chemical and electrostatic studies of anionic water clusters, $(H_2O)_n^-$	A. D. Kulkarni S. R. Gadre S. Nagase	J. Theor. Comp. Chem. **851**, 213 (2008)
181. Molecular electrostatic potentials of divalent carbon(0) compounds	M. M. Deshmukh S. R. Gadre R. Tonner G. Frenking	Phys. Chem. Chem. Phys. **10**, 2298 (2008)

182. Structure, energetics and reactivity of boric acid nanotubes: A molecular tailoring approach	M. Elango V. Subramanian A. P. Rahalkar S. R. Gadre N. Sathyamurthy	J. Phys. Chem. A **112**, 7699 (2008)
183. Cation-π interaction: to stack or to spread	B. K. Mishra V. K. Bajpai V. Ramanathan S. R. Gadre N. Sathyamurthy	Mol. Phys. **106**, 1557 (2008)
184. Electrostatic guidelines and molecular tailoring for density functional investigation of structures and energetics of $(Li)_n$ clusters	K. V. Jovan Jose S. R. Gadre	J. Chem. Phys. **129,** 164314 (2008)
185. An appraisal of Poincare–Hopf relation and application to topography of molecular electrostatic potentials	D. Roy P. Balanarayan S. R. Gadre	J. Chem. Phys. **129**, 174103 (2008)
186. Use of molecular electrostatic potential for quantitative assessment of inductive effect	C. H. Suresh P. Alexander K. P. Vijayalaxmi P. K. Sajith S. R. Gadre	Phys. Chem. Chem. Phys. **10**, 6492 (2008)
187. Enabling *ab initio* hessian and frequency calculations of large molecules	A. P. Rahalkar V. Ganesh S. R. Gadre	J. Chem. Phys. **129**, 234101 (2008)
188. Atoms and molecules : A momentum space perspective	P. Balanarayan S. R. Gadre	A chapter in **Chemical Reactivity Theory: A Density Functional View**, Ed. P. K. Chattaraj, CRC Press (2009), pp. 55-70
189. Web MTA: A Web-Interface for *ab initio* geometry optimization of large molecules using molecular tailoring approach	R. K. Kavathekar S. Khire V. Ganesh A. P. Rahalkar S. R. Gadre	J. Comp. Chem. **30**, 1167 (2009)

190. Significant progress in predicting the crystal structures of small organic molecules – a report on the fourth blind test	G. M. Day T. G. Cooper A. J. Cruz-Cabeza K. E. Hejczyk H. L. Ammon S. X. M. Boerrigter J. S. Tan R. G. Della Valle E. Venuti K.V. Jovan Jose S. R. Gadre, *et al.*	Acta Cryst. B**65**, 107 (2009)
191. *Ab initio* study on $(CO_2)_n$ clusters via electrostatics- and molecular tailoring-based algorithm	K. V. Jovan Jose S. R. Gadre	Intern. J. Quantum Chem. **109**, 2238 (2009)
192. Estimation of N-H· · ·O=C intermolecular hydrogen bond energy in polypeptides	M. M. Deshmukh S. R. Gadre	J. Phys. Chem. A **113**, 7927 (2009)
193. Signatures of molecular recognition from the topography of electrostatic potential	D. K. Roy P. Balanarayan S. R. Gadre	J. Chem. Sci. **121**, 815 (2009)
194. Stepwise hydration of protonated carbonic acid: A theoretical study	M. Prakash V. Subramanian S. R. Gadre	J. Phys. Chem. A **113**, 1260 (2009)
195. Molecular tailoring approach for exploring structures, energetics and properties of clusters	S. R. Gadre K. V. Jovan Jose A. P. Rahalkar	J. Chem. Sci. **122**, 47 (2010)
196. On the applicability of fragmentation methods to conjugated π systems within Density Functional Framework	S. D. Yeole S. R. Gadre	J. Chem. Phys. **132**, 094102 (2010)
197. Molecular tailoring approach in conjunction with MP2 and RI-MP2 codes: A comparison with fragment molecular method	A. P. Rahalkar M. Katouda S. R. Gadre S. Nagase	J. Comput. Chem. **31**, 2405 (2010)
198. A Density Functional Investigation on the Structures, Energetics and Properties of Sodium Clusters through Electrostatic Guidelines and Molecular Tailoring	K. V. Jovan Jose S. S. Khire S. R. Gadre	A chapter in a **Aromaticity and Metal Clusters**, Ed. P. Chattaraj, Taylor & Francis / CRC Press (India) (2010), p. 205- 226

199. Appraisal of through-bond and through-space substituent effects via molecular electrostatic potential topography	F. B. Sayyad C. H. Suresh S. R. Gadre	J. Phys. Chem. A **114**, 12330 (2010)
200. *Ab Initio* Investigation of Benzene Clusters: Molecular Tailoring Approach	A. S. Mahadevi A. P. Rahalkar S. R. Gadre G. N. Sastry	J. Chem. Phys. **133**, 164308 (2010)
201. Molecular Tailoring: An Art of the Possible for Ab Initio Treatment of Large Molecules and Molecular Clusters	A. P. Rahalkar S. D. Yeole V. Ganesh S. R. Gadre	A Chapter in **Linear-Scaling Techniques in Computational Chemistry and Physics**, Ed. R. Zaleśny, M.G. Papadopoulos, P.G. Mezey and J. Leszczynski, Springer (2011), p. 199-225
202. Molecular Cluster Building Algorithm : Electrostatic Guidelines and Molecular Tailoring Approach	S. D. Yeole S. R. Gadre	J. Chem. Phys. **134**, 084111 (2011)
203. Estimation of hydrogen bond energies in α, β and γ cyclodextrins	M. M. Deshmukh L. J. Bartolotti S. R. Gadre	J. Comp. Chem. **32**, 2996 (2011)
204. Topography of Scalar Fields: Molecular Clusters and π-Conjugated Systems,	S. D. Yeole S. R. Gadre	J. Phys. Chem. A, **115**, 12769 (2011). (Invited article in a special issue honoring Prof. R. F. W. Bader)
205. "Gold standard" coupled-cluster study of acetylene pentamers and hexamers via molecular tailoring approach	A. P. Rahalkar B. K. Mishra V. Ramanathan S. R. Gadre	Theor. Chem. Acc. **130**, 491 (2011) (Invited article in a special issue honoring Prof. S. Nagase)
206. Acetylene Aggregates via Cluster Building Algorithm and Molecular Tailoring Approach	A. P. Rahalkar S. D. Yeole S. R. Gadre	Theor. Chem. Acct. **131**, 1095 (2012) (Invited article in a special issue honoring Prof. E. D. Jemmis)
207. Tailoring Approach for obtaining Molecular Orbitals for Large Systems	A. P. Rahalkar S. R. Gadre	J. Chem. Sci. **124**, 149 (2012)
208. Structures, Energetics and Vibrational Spectra of CO_2 Clusters through Molecular Tailoring and Cluster Building Algorithm	S. D. Yeole N. Sahu S. R. Gadre	Phys. Chem. Chem. Phys. **14**, 7718 (2012)

209. Hydrogen bond energies and cooperativity in substituted calix[n]arenes (n=4, 5)	J. K. Khedkar M. M. Deshmukh S. R. Gadre S. P. Gejji	J. Phys. Chem. A **116**, 3739 (2012)
210. Studies toward Oxyacetamide-Linked RNA Analogues: Synthesis and Conformation of a Modified Dinucleoside	A. M. Jabgunde S. D. Yeole S. P. Sanap S. R. Gadre D. D. Dhavale	Synthesis **44**, 2277 (2012)
211. Facilitating Minima Search for Large Water Clusters at MP2 Level via Molecular Tailoring	J. P. Furtado Anuja P. Rahalkar S. Shanker P. Bandyopadhyay S. R. Gadre	J. Phys. Chem. Lett. **3**, 2253 (2012)
212. Rapid Topography Mapping of Scalar Fields: Large Molecular Clusters	S. D. Yeole R.Lopez S. R. Gadre	J. Chem. Phys. **137**, 074116 (2012)
213. Appraisal of Molecular Tailoring Approach for Large Clusters	N. Sahu S. D. Yeole S. R. Gadre	J. Chem. Phys. **138**, 104101 (2013)
214. High-Level Ab Initio Investigations on Structures and Energetics of N_2O Clusters	S. D. Yeole N. Sahu S. R. Gadre	J. Phys. Chem. A **117**, 8591 (2013)
215. Stabilization of Si(0) and Ge(0) Compounds by Different Silylenes and Germylenes: A Density Functional and Molecular Electrostatic Study	S. Sarmah A. K. Guha A. K. Phukan A. Kumar S. R. Gadre	Dalton Trans. **42**, 13200 (2013)
216. Molecular electrostatics for probing lone pair–π interactions	N. Mohan C. H. Suresh, A. Kumar S. R. Gadre	Phys. Chem. Chem. Phys. **15**, 18401 (2013)
217. Exploring structures and energetic of large OCS clusters by correlated methods	N. Sahu G. Singh S. R. Gadre	J. Phys. Chem. A **42**, 117 (2013)
218. Lone pairs: An Electrostatic Viewpoint	A. Kumar S. R. Gadre N. Mohan C. H. Suresh	J. Phys. Chem. A 2014