

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

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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**, 613 (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 wavefunctions  
S. R. Gadre  
P. T. Narasimhan  
Intern. J. Quantum Chem. **12**, 105 (1977)
6. Electron momentum distributions and Compton profiles from FSGO wavefunctions  
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 wavefunctions  
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<br>S. R. Gadre                      | J. Chem. Phys. <b>72</b> , 3669<br>(1980)                |
| 12. Electronegativities of the element from simple X-alpha theory  | L. J. Bartolotti<br>S. R. Gadre<br>R.G. Parr   | J. Amer. Chem. Soc. <b>102</b> ,<br>2945 (1980)          |
| 13. Bounds for Coulomb energies  | S. R. Gadre<br>N. H. Handy<br>L. J. Bartolotti | J. Chem. Phys. <b>72</b> , 1034<br>(1980)                |
| 14. Theoretical Compton profile anisotropies in molecules and solids - VIII. Vibrational and rotational dependence of Compton profiles | B.M. Pettitt<br>S. R. Gadre<br>R.L. Matcha     | Intern. J. Quantum Chem.<br>Symp. <b>14</b> , 697 (1980) |
| 15. An information theoretic synthesis and analysis of Compton profiles  | S. B. Sears<br>S. R. Gadre                     | J. Chem. Phys. <b>75</b> , 4626<br>(1981)                |
| 16. Direct and reverse transformations between electron density and electron momentum density  | S. R. Gadre<br>R. K. Pathak                    | Phys. Rev. <b>A24</b> , 2906<br>(1981)                   |
| 17. Estimation of $\langle p \rangle$ and $\langle 1/p \rangle$ from atomic electron densities   | R.K. Pathak<br>S. R. Gadre                     | J. Chem. Phys. <b>74</b> , 5925<br>(1981)                |
| 18. On representation of the Coulomb integral by one-electron functionals  | S. R. Gadre<br>R. K. Pathak                    | J. Chem. Phys. <b>75</b> , 4740<br>(1981)                |
| 19. Inequalities among atomic expectation values   | S. R. Gadre<br>R. L. Matcha                    | J. Chem. Phys. <b>74</b> , 589<br>(1981)                 |
| 20. Novel DNA sequence organization in rice genome   | V. Gupta<br>S. R. Gadre<br>P. K. Ranjekar      | Biochem. Biophys. Acta<br><b>656</b> , 147 (1981)        |
| 21. On the monotonicity of atomic momentum densities and inequalities among atomic expectation values                                  | S. R. Gadre<br>R. L. Matcha                    | J. Chem. Phys. <b>76</b> , 748<br>(1982)                 |

- |  |   |   |
|--|---|---|
| 22. Estimation of $\langle p \rangle$ and $\langle 1/p \rangle$ from atomic densities : A comment  | S. R. Gadre<br>R. K. Pathak                   | J. Chem. Phys. <b>77</b> , 1073<br>(1982)             |
| 23. Estimation of $\langle r^n \rangle$ -values from atomic momentum densities   | S. R. Gadre<br>S. P. Gejji<br>N. Venkatalaxmi | Phys. Rev. <b>A26</b> , 1768<br>(1982)                |
| 24. A local density functional model in momentum space   | R.K. Pathak<br>P. V. Panat<br>S. R. Gadre     | Phys. Rev. <b>A26</b> , 3073<br>(1982)                |
| 25. Lower bounds to the Weizsäcker correction  | S. R. Gadre<br>R. K. Pathak                   | Phys. Rev. <b>A25</b> , 668<br>(1982)                 |
| 26. Relationships between the terms in the gradient expansion : Kinetic and exchange energy functionals                                    | R. K. Pathak<br>S. R. Gadre                   | Phys. Rev. <b>A25</b> , 3426<br>(1982)                |
| 27. A study on monotonicity and shell structure characteristics of atomic electron momentum densities                                      | S.R. Gadre<br>R.K. Pathak<br>S. Chakravorty   | J. Chem. Phys. <b>78</b> , 4581<br>(1983)             |
| 28. Hartree-Fock momentum expectation values of atoms and ions   | S. R. Gadre<br>S. P. Gejji<br>S. Chakravorty  | At. Data Nucl. Data<br>Tables <b>28</b> , 477 (1983). |
| 29. Direct and reverse transformations between electron density and electron momentum density :connection with the locally averaged method | S. R. Gadre<br>S. P. Gejji<br>R. K. Pathak    | Phys. Rev. <b>A28</b> , 462<br>(1983)                 |
| 30. Electron density to electron momentum density : The use of an energy constraint  | S. R. Gadre<br>S. P. Gejji<br>R. K. Pathak    | Phys. Rev. <b>A27</b> , 3328<br>(1983)                |
| 31. Representation of electron repulsion energies energy by simple one-electron functionals  | S. R. Gadre<br>R. D. Bendale                  | J. Chem. Phys. <b>78</b> , 996<br>(1983)              |

- |  |   |  |
|--|---|--|
| 32. Gradient-free representation of the Weizsäcker term for atoms  | R.K. Pathak<br>S.R. Gadre                   | Phys. Rev. <b>A28</b> , 1808<br>(1983)                 |
| 33. Use of energy constraint for refinement of electron momentum densities   | S. R. Gadre<br>S. P. Gejji                  | J. Chem. Phys. <b>80</b> , 175<br>(1984)               |
| 34. From molecular electron density to electron momentum densities   | R.K. Pathak<br>S. P. Gejji<br>S. R. Gadre   | Phys. Rev. <b>A29</b> , 3402<br>(1984)                 |
| 35. Extraction of molecular electron momentum densities from electron density contour maps   | S. R. Gadre<br>S. P. Gejji                  | Chem. Phys. Letters <b>112</b> ,<br>45 (1984)          |
| 36. Information entropy and Thomas Fermi theory  | S.R. Gadre                                  | Phys. Rev. <b>A30</b> , 620<br>(1984)                  |
| 37. Refinement of electron momentum densities of ionic solids using an experimental energy constraint  | S. R. Gadre<br>S. P. Gejji                  | Chem. Phys. Letters <b>109</b> ,<br>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<br>M. Lagu<br>S. R. Gadre          | Ind. J. Biochem. and<br>Biophys. <b>21</b> , 81 (1984) |
| 39. The self interaction correction to the local spin density model : Effect on atomic momentum space properties                                 | S. R. Gadre<br>S. J. Chakravorty            | Chem. Phys. Letters <b>120</b> ,<br>101 (1985)         |
| 40. Analysis of atomic electron momentum densities : use of information entropies in coordinate and momentum space                               | S. R. Gadre<br>R. D. Bendale<br>S. P. Gejji | Chem. Phys. Letters <b>17</b> ,<br>138 (1985)          |
| 41. Maximization of atomic information entropy sum in configuration and momentum spaces  | S. R. Gadre<br>R. D. Bendale                | Intern. J. Quantum Chem.<br><b>28</b> , 311 (1985)     |
| 42. Information entropies in quantum chemistry   | S. R. Gadre<br>R. D. Bendale                | Curr. Sci.(India) <b>54</b> ,970<br>(1985)             |

- |  |  |   |
|--|--|---|
| 43. Some novel characteristics of atomic information entropies   | S. R. Gadre<br>S. B. Sears<br>S. J. Chakravorty<br>R. D. Bendale | Phys. Rev. <b>A32</b> , 2602<br>(1985)                            |
| 44. A novel approach for the study of interactions : molecular electron densities  | T. N. Guru Row<br>S. R. Gadre                                    | Proc. Ind. Acad. Sci.<br>(Chem. Sci.). <b>95</b> , L437<br>(1985) |
| 45. Electron density in chemistry  | S. R. Gadre  | Curr. Sci. <b>54</b> , 329 (1985)                                 |
| 46. Interconnections between atomic electron density and electron momentum density : leading and tail correction                   | S. R. Gadre<br>S. J. Chakravorty                                 | Phys. Rev. <b>A33</b> , 1374<br>(1986)                            |
| 47. Compton profiles of atoms from electron density via reciprocal form factors  | S. R. Gadre<br>S. J. Chakravorty                                 | Proc. Ind. Acad. Sci.<br>(Chem. Sci.) <b>96</b> , 241<br>(1986)   |
| 48. Some rigorous inequalities among the Weizsäcker correction, $\langle r^n \rangle$ and $\langle p^n \rangle$ expectation values | S. R. Gadre<br>S.J. Chakravorty                                  | J. Chem. Phys. <b>84</b> , 7051<br>(1986)                         |
| 49. Average electron momentum densities and rigorous bounds to average electron densities for atoms and molecules                  | S. R. Gadre<br>S. J. Chakravorty                                 | Chem. Phys. Letters <b>132</b> ,<br>535 (1986)                    |
| 50. On the similarity between molecular electron densities, electrostatic potentials and bare-nuclear potentials                   | S. R. Gadre<br>R. D. Bendale                                     | Chem. Phys. Letters <b>130</b> ,<br>515 (1986)                    |
| 51. Use of a nonlocal density approximation for the transformation of atomic electron density to electron momentum density         | S. R. Gadre<br>S. J. Chakravorty                                 | J. Chem. Phys. <b>86</b> , 2224<br>(1987)                         |
| 52. Coulomb energy, total X-ray scattering intensities and average electron densities  | S. J. Chakravorty<br>S. R. Gadre                                 | Chem. Phys. Letters <b>142</b> ,<br>205 (1987)                    |
| 53. Nonlocal-density approximation for exploring kinetic energy anisotropies   | S. R. Gadre<br>T. Koga<br>S. J. Chakravorty                      | Phys. Rev. <b>A36</b> , 4155<br>(1987)                            |

- |   |  |  |
|---|--|--|
| 54. Rigorous relationships among quantum mechanical kinetic energy and information entropies : upper and lower bounds | S. R. Gadre<br>R. D. Bendale                       | Phys. Rev. <b>A36</b> , 1932<br>(1987)   |
| 55. Use of second-moment constraint for the refinement of determinantal wave function                                 | S. R. Gadre<br>S. A. Kulkarni<br>I. H. Shrivastava | Phys. Rev. <b>A38</b> , 487<br>(1988)  |
| 56. Property-oriented basis-sets using cross-entropy minimization   | S. R. Gadre<br>S. A. Kulkarni<br>I. H. Shrivastava | Portugalea Fisica <b>19</b> , 349<br>(1988)  |
| 57. Bounds to electron repulsion energies   | S. R. Gadre<br>R. K. Pathak                        | Proc. Ind. Acad. Sci.<br>(Chem. Sci.) <b>100</b> , 483<br>(1988)   |
| 58. Development of links between electron densities in complementary spaces   | R. K. Pathak<br>S. R. Gadre                        | Portugalea Fisica <b>19</b> , 407<br>(1988)  |
| 59. Rigorous bounds to molecular electron repulsion and electrostatic potential integrals                             | S. R. Gadre<br>S. A. Kulkarni<br>R. K. Pathak      | J. Chem. Phys. <b>91</b> , 3596<br>(1989)  |
| 60. Reduced first-order density matrices and exchange-only correlation factors for closed-shell atomic systems        | S. R. Gadre<br>S. A. Kulkarni<br>R. K. Pathak      | Phys. Rev. <b>A40</b> , 4224<br>(1989)   |
| 61. Interconnections between electron densities in position and momentum spaces                                       | S. R. Gadre<br>R. K. Pathak                        | A Chapter in a book:<br>Aspects of many body<br>effects in molecules and<br>extended systems, Ed. D.<br>Mukherjee, Lecture notes<br>in Chem. Vol. <b>50</b> ,<br>Springer (1989) |
| 62. Atomic and molecular diamagnetic susceptibilities from Compton scattering data                                    | S. R. Gadre<br>R. K. Pathak                        | J. Chem. Phys. <b>92</b> , 4327<br>(1990)  |
| 63. Momentum space atomic first-order density matrices and 'exchange-only' correlation factors                        | R. K. Pathak<br>S. A. Kulkarni<br>S. R. Gadre      | Phys. Rev. <b>A42</b> , 2622<br>(1990)   |

- |  |  |   |
|--|--|---|
| 64. Cross-entropy minimization for refinement of Gaussian basis-sets   | S. R. Gadre<br>S. A. Kulkarni<br>I. H. Shrivastava                 | Chem. Phys. Letters <b>166</b> ,<br>445 (1990)                              |
| 65. Applications of rigorous bounds for efficient evaluation of molecular electrostatic potentials                                     | S. R. Gadre<br>I. H. Shrivastava<br>S. A. Kulkarni                 | Chem. Phys. Letters <b>170</b> ,<br>271 (1990)                              |
| 66. Nonexistence of local maxima in molecular electrostatic potential maps   | S. R. Gadre<br>R. K. Pathak  | Proc. Ind. Acad. Sci.<br>(Chem. Sci.) <b>102</b> , 189<br>(1990)            |
| 67. Maximal and minimal characteristics of molecular electrostatic potentials  | R. K. Pathak<br>S. R. Gadre  | J. Chem. Phys. <b>93</b> , 1770<br>(1990)                                   |
| 68. A general parallel algorithm for the generation of molecular electrostatic potential maps  | S. R. Gadre<br>S. V. Bapat<br>K. Sundararajan<br>I. H. Shrivastava | Chem. Phys. Letters <b>175</b> ,<br>307 (1990)                              |
| 69. Some investigations on symmetry and extremal properties of molecular electron momentum densities                                   | S. R. Gadre<br>A. C. Limaye<br>S. A. Kulkarni                      | J. Chem. Phys. <b>94</b> , 8040<br>(1991)                                   |
| 70. Computation of molecular electrostatic potential : efficient algorithm and parallelization   | S. R. Gadre<br>S. Bapat<br>I. H. Shrivastava                       | Comp. And Chem. <b>15</b> ,<br>203 (1991)                                   |
| 71. Reply to the comment on the paper "Maximal and minimal characteristics of molecular electrostatic potentials" : further extensions | S. R. Gadre<br>S. A. Kulkarni<br>R. K. Pathak                      | J. Chem. Phys. <b>94</b> , 8639<br>(1991)                                   |
| 72. Some aspects of parallelization of two-electron integrals in molecular orbital programs  | S. R. Gadre<br>S. A. Kulkarni<br>A. C. Limaye<br>R. N. Shirsat     | Zeit. Phys. - D :Atoms,<br>Molecules and Clusters<br><b>18</b> , 357 (1991) |
| 73. Shapes and sizes of molecular anions via topographical analysis of electrostatic potential   | S. R. Gadre<br>I. H. Shrivastava                                   | J. Chem. Phys. <b>94</b> , 4384<br>(1991)                                   |

- |   |  |   |
|---|--|---|
| 74. Parallelization of two electron integrals in molecular orbital programs                             | S. R. Gadre<br>S. A. Kulkarni<br>A. C. Limaye<br>A. Taspaa | A Chapter in <i>Advanced Computing</i> , p. 388-391<br>Ed. V. P. Bhatkar, Tata Mc Graw Hill (1991)  |
| 75. Algorithm development and parallelization of molecular electrostatic potential                      | S. R. Gadre<br>S. Bapat<br>I. Shrivastava                  | A Chapter in <i>Advanced Computing</i> , p. 388-391<br>Ed. V. P. Bhatkar, Tata Mc Graw Hill (1991). |
| 76. Bounds to atomic and molecular energy functionals   | S. R. Gadre<br>R. K. Pathak                                | Adv. Quantum Chem. <b>22</b> , 211, Ed. P.-O. Löwdin, Academic, New York (1991)                     |
| 77. Molecular electrostatic potentials: a topographical study   | S. R. Gadre<br>S. A. Kulkarni<br>I.H. Shrivastava          | J. Chem. Phys. <b>96</b> , 5253 (1992)  |
| 78. Deriving chemical parameters from molecular electrostatic potential maps of molecular anions        | S. R. Gadre<br>C. Koimel<br>I. H. Shrivastava              | Inorg. Chem. <b>31</b> , 2279 (1992)  |
| 79. Topographical view of molecular electron momentum densities.  | S. A. Kulkarni<br>S. R. Gadre<br>R. K. Pathak              | Phys. Rev. <b>A45</b> , 4399 (1992)   |
| 80. Molecular electrostatics of $[V_{10}O_{28}]^-$ cluster : a graphics visualization study using PARAM | S. R. Gadre<br>S. Bapat<br>A. Taspaa<br>R. N. Shirsat.     | Curr. Sci. (India) <b>62</b> , 798 (1992)   |
| 81. Molecular electrostatics: A comprehensive topographical approach.                                   | R. N. Shirsat<br>S. V. Bapat<br>S. R. Gadre.               | Chem. Phys. Letters <b>200</b> , 373 (1992)   |
| 82. Development of a restricted Hartree-Fock program INDMOL on PARAM: A highly parallel computer.       | R. N. Shirsat<br>A. C. Limaye<br>S. R. Gadre.              | J. Comput. Chem <b>14</b> , 445 (1993)  |
| 83. Density based localisation function via nonlocal density approximation.                             | S. R. Gadre<br>S. A. Kulkarni<br>R. K. Pathak              | J. Chem. Phys. <b>98</b> , 3574 (1993)  |
| 84. Visualization of shapes of molecular anions   | S. R. Gadre<br>C. Kölmel<br>M. Ehrig<br>R. Ahlrichs        | Z. Naturforsch. -A <b>48</b> , 137 (1993)   |

- |  |  |  |
|--|--|--|
| 85. On the topography of electron momentum densities of linear molecules   | S. A. Kulkarni<br>S. R. Gadre  | Z. Naturforsch. -A <b>48</b> , 145 (1993)                  |
| 86. Momentum space investigation of $C_{2v}$ dissociation of water   | S. R. Gadre<br>S. A. Kulkarni  | Proc. Ind. Acad. Sci. (Chem. Sci.) <b>105</b> , 149 (1993) |
| 87. Topography driven electrostatic charge models for molecules  | S. R. Gadre<br>I. H. Shrivastava   | Chem. Phys. Letters <b>205</b> , 350 (1993)                |
| 88. Probing chemical reactions in momentum space   | S. A. Kulkarni<br>S. R. Gadre  | J. Amer. Chem. Soc. <b>115</b> , 7434 (1993)               |
| 89. Radii of monpositive atomic ions   | S. R. Gadre<br>K. D. Sen   | J. Chem. Phys. <b>99</b> , 3149 (1993)                     |
| 90. SCRF calculation of the effect of water on the topology of molecular electrostatic potential   | F. J. Luque<br>M. Orozco<br>P.K. Bhadane<br>S. R. Gadre                                      | J. Phys. Chem. <b>97</b> , 9380 (1993)                     |
| 91. Molecular electrostatic charge models: a topographical approach.   | I. H. Shrivastava<br>S. R. Gadre   | Intern. J. Quantum Chem. <b>49</b> ,397 (1994)             |
| 92. Graphics visualization of molecular surfaces   | S. R. Gadre<br>A. Taspaa   | J. Mol. Graphics <b>12</b> , 45 (1994)                     |
| 93. Electrophilic additions to 7-methylenenorbornenes and 7-isopropylidenenorbornenes: can remote substituents swamp electrostatic control of $\pi$ -face selectivity? | G. Mehta<br>G. Gunasekaran<br>S. R. Gadre<br>R. N. Shirsat<br>B. Ganguly<br>J. Chandrasekhar | J. Org. Chem. <b>59</b> , 1953 (1994)                      |
| 94. Electrostatic vs orbital control of $\pi$ - face selectivities: experimental and theoretical study of electrophilic additions to 7-isopropylidene norbornanes.     | G. Mehta<br>F. A. Khan<br>S. R. Gadre<br>R. N. Shirsat<br>B. Ganguly<br>J. Chandrasekhar     | Angew. Chem. Int. Ed. Engl. <b>33</b> , 1390 (1994)        |
| 95. A general parallel solution to the integral transformation and MP2 energy evaluation on distributed memory parallel machines                                       | A. C. Limaye<br>S. R. Gadre  | J. Chem. Phys. <b>100</b> , 1303 (1994)                    |
| 96. Comment on "Computing molecular electrostatic potentials with PRISM algorithm" by Johnson, Gill, Pople and Fox   | S. R. Gadre<br>R. N. Shirsat   | Chem. Phys. Letters <b>218</b> , 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<sub>60</sub> 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 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 cyclobutabenzene  
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 localisation 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 the 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 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, p. 219-522, Ed. J. Murray and K. D. Sen, Elsevier, Amsterdam (1996)
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<sub>60</sub> 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 co-ordination: CF<sub>3</sub>SO<sub>3</sub><sup>-</sup> ion as a test 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 <i>ab initio</i> theoretical study                         | A. K. Bhattacharya<br>S. S. Pundlik<br>S. R. Gadre   | Cancer Investigation <b>15</b> ,<br>531 (1997)  |
| 120. Electrostatic investigation of metal cation binding to DNA bases and base pairs  | S. S. Pundlik<br>S. R. Gadre<br>A. C. Limaye<br>A. P. Rendell                                    | Chem. Commun. 573<br>(1998)                     |
| 121. Novel electrostatic approach to substituent constants: doubly substituted benzenes   | C. H. Suresh<br>S. R. Gadre  | J. Amer. Chem. Soc. <b>120</b> ,<br>7049 (1998) |
| 122. Face selectivity in electrophilic additions to methylenenorbornanes: relative importance of through-space, through-bond and electrostatic interactions | G. Mehta<br>C. Ravikrishna<br>S. R. Gadre<br>C. H. Suresh<br>P. Kalyanaraman<br>J. Chandrasekhar | Chem. Commun. 975<br>(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<br>S. R. Gadre<br>S. P. Gejji   | Theor. Chem. Acc. <b>99</b> ,<br>151 (1998)     |
| 124. Polarization corrected electrostatic potential for probing cation binding patterns of molecules 1. Saturated hydrocarbons                              | S. R. Gadre<br>S. S. Pingale   | J. Amer. Chem. Soc. <b>120</b> ,<br>7056 (1998) |
| 125. Complexes of ammonia with propane and cyclopropane: electrostatic guidelines for <i>ab initio</i> treatment  | S. R. Gadre<br>P. K. Bhadane   | Theor. Chem. Acc. <b>100</b> ,<br>300 (1998)    |
| 126. Co-operative electrostatics for understanding crown ether hydration patterns   | S. R. Gadre<br>S. S. Pingale   | Curr. Sci. (India) <b>75</b> , 1162<br>(1998)   |
| 127. Electrostatic insights into molecular hydration process: a case study of crown ethers  | S. S. Pingale<br>S. R. Gadre<br>L. J. Bartolotti   | J. Phys. Chem. <b>A102</b> ,<br>9987 (1998)     |
| 128. Clar's aromatic sextet theory revisited via molecular electrostatic potential topography   | C. H. Suresh<br>S. R. Gadre  | J. Org. Chem. <b>64</b> , 2505<br>(1999)        |
| 129. Molecular electrostatics for exploring complexes of carbonyl compounds with hydrogen fluoride  | S. R. Gadre<br>P. K. Bhadane   | J. Phys. Chem. <b>A103</b> ,<br>3512 (1999)     |

130. Electrostatics in chemistry. 1 Basic principles  
S. R. Gadre  
P. K. Bhadane  
Resonance **4(2)**, 11 (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  $(\text{CF}_3\text{SO}_2)_2\text{N}^-\text{Li}^+$  ion pairs  
S. P. Gejji  
C. H. Suresh  
K. Babu  
S. R. Gadre  
J. Phys. Chem. **A103**, 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**, p. 1-53, Ed. Jerzy Leszczynski, World Scientific, Singapore (1999)
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. **A39**, 50 (2000)
137. Molecular electrostatic potential and electron density topography: structure and reactivity of (substituted arene)  $\text{Cr}(\text{CO}_3)$  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 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 compensive 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<sup>+</sup>(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<sub>2</sub>O)<sub>n</sub>, 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- $\pi$  Complexes of acetylene-ethylene: a matrix Isolation and Computational Study  
K. Sundararajan  
K. Sankaran  
K. S. Vishwanathan  
A. D. Kulkarni  
S. R. Gadre  
J. Phys. Chem. A **106**, 1504 (2002)
147. H... $\pi$  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 dimer of naphthalene & 2-cyanonaphthalene in a supersonic jet   | A. Das<br>K. K. Mahato<br>C. K. Nandi<br>T. Chakraborty<br>S. R. Gadre<br>N. A. Gokhale | Phys. Chem. Chem. Phys. <b>4</b> , 2162 (2002)  |
| 149. Electrophilic additions to a 2-methylenebicyclo [2.1.1] hexane system: Probing $\pi$ -face selectivity for electrostatic and orbital effects | G. Mehta<br>S. R. Singh<br>P. Balanarayan<br>S. R. Gadre                                | Org. Lett. <b>4</b> , 2297 (2002)   |
| 150. <i>Ab initio</i> quality one-electron properties of large molecules: development and testing of molecular tailoring approach                 | K. Babu<br>S. R. Gadre  | J. Comput. Chem. <b>24</b> , 484 (2003)   |
| 151. Information theoretical approaches to quantum chemistry  | S. R. Gadre   | Reviews of Modern Quantum Chemistry : A Celebration of the Contributions of Robert G. Parr, Vol. <b>1</b> , p. 108-147, Ed. K. D. Sen, World Scientific, Singapore (2003) |
| 152. Topography of molecular scalar fields. I. Algorithm and Poincare-Hopf relation   | P. Balanarayan<br>S. R. Gadre   | J. Chem. Phys. <b>119</b> , 5037 (2003)   |
| 153. Electrostatics-guided <i>Ab initio</i> studies on weakly bonded complexes of substituted naphthalenes  | S. R. Gadre<br>M. M. Deshmukh<br>T. Chakraborty   | Chem. Phys. Lett. <b>384</b> , 350 (2004)   |
| 154. Exploring hydration patterns of aldehydes and amides : <i>Ab initio</i> investigations   | A. D. Kulkarni<br>K. Babu<br>S. R. Gadre<br>L. J. Bartolotti                            | J. Phys. Chem. A <b>108</b> , 2492 (2004)   |
| 155. Tailoring approach for exploring electron densities and electrostatic potentials of molecular crystals                                       | K. Babu<br>V. Ganesh<br>S. R. Gadre<br>N. E. Ghermani                                   | Theor. Chem. Acc. <b>111</b> , 255 (2004)   |
| 156. Many body interaction analysis: Algorithm development and applications to large molecular clusters   | A. D. Kulkarni<br>V. Ganesh<br>S. R. Gadre  | J. Chem. Phys. <b>121</b> , 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  
Thematic Professor P. T. Narasimhan festschrift Issue : Proceedings of Indian National Science Academy **70A**, 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  
"Recent Trends in Practice and Theory of Information Technology: Proceedings of NRB Seminar", Editor S. N. Maheshwari, Viva Books, 298 (2005)
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)
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 tailoring approach : Towards PC-based *ab initio* treatment of large molecules  
S. R. Gadre  
V. Ganesh  
J. Theor. Comp. Chem. (*in press* 2005)