# Shridhar R Gadre

List of Publications by Year
in descending order

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|---|---|---|---|
| 214 papers | 8,529 citations | 34105 52 h-index | 58581 82 g-index |
| 215 all docs | 215 docs citations | 215 times ranked | 3957 citing authors |

| # | Article | IF | Citations |
|---|---|---|---|
| 1 | Enabling Rapid and Accurate Construction of CCSD(T)-Level Potential Energy Surface of Large Molecules Using Molecular Tailoring Approach. Journal of Physical Chemistry A, 2022, 126, 1458-1464. | 2.5 | 7 |
| 2 | Development and testing of an algorithm for efficient MP2/CCSD(T) energy estimation of molecular clusters with the 2â€“body approach. Journal of Computational Chemistry, 2022, , . | 3.3 | 0 |
| 3 | Hydration shell model for expeditious and reliable individual hydrogen bond energies in large water clusters. Physical Chemistry Chemical Physics, 2022, 24, 15462-15473. | 2.8 | 8 |
| 4 | DAMQT 3: Advanced suite for the analysis of molecular density and related properties in large systems. Computer Physics Communications, 2022, 279, 108460. | 7.5 | 2 |
| 5 | Citation-Based Criterion for Identifying Long-Lasting Research Papers. Current Science, 2021, 120, 209. | 0.8 | 0 |
| 6 | Molecular Tailoring Approach for the Estimation of Intramolecular Hydrogen Bond Energy. Molecules, 2021, 26, 2928. | 3.8 | 30 |
| 7 | Electrostatic Potential Topology for Probing Molecular Structure, Bonding and Reactivity. Molecules, 2021, 26, 3289. | 3.8 | 79 |
| 8 | Life and Science of Clemens C. J. Roothaan. Resonance, 2021, 26, 737-755. | 0.3 | 2 |
| 9 | Antiaromaticityâ€“Aromaticity Interplay in Fused Benzenoid Systems Using Molecular Electrostatic Potential Topology. Journal of Physical Chemistry A, 2021, 125, 5999-6012. | 2.5 | 10 |
| 10 | Molecular Tailoring Approach for Estimating Individual Intermolecular Interaction Energies in Benzene Clusters. Journal of Physical Chemistry A, 2021, 125, 6131-6140. | 2.5 | 16 |
| 11 | Theoretical and experimental study of IR spectra of large phenol-acetylene clusters, Ph(Ac)n for 8 â‰¤ n â‰¤ 12. Journal of the Indian Chemical Society, 2021, 98, 100100. | 2.8 | 2 |
| 12 | Unusually Large Hydrogen-Bond Cooperativity in Hydrogen Fluoride Clusters, (HF)<sub>n</sub>,n= 3 to 8, Revealed by the Molecular Tailoring Approach. Journal of Physical Chemistry A, 2021, 125, 8836-8845. | 2.5 | 16 |
| 13 | Direct and Reliable Method for Estimating the Hydrogen Bond Energies and Cooperativity in Water Clusters, W<sub>n</sub>, n = 3 to 8. Journal of Physical Chemistry A, 2020, 124, 6699-6706. | 2.5 | 34 |
| 14 | Fragmentation method reveals a wide spectrum of intramolecular hydrogen bond energies in antioxidant natural products. New Journal of Chemistry, 2020, 44, 5841-5849. | 2.8 | 12 |
| 15 | Eleven Years of Dr D. S. Kothari Postdoctoral Fellowship Scheme of the University Grants Commission. Current Science, 2020, 118, 352. | 0.8 | 0 |
| 16 | Electrostatic Topographical Viewpoint of Ï€-Conjugation and Aromaticity of Hydrocarbons. Journal of Physical Chemistry A, 2019, 123, 10139-10151. | 2.5 | 9 |
| 17 | Electrostatics-Assisted Building-Up Procedure for Capturing Energy Minima of Metal Clusters: Test Case of Ag<sub>n</sub> Clusters. Journal of Physical Chemistry A, 2019, 123, 7872-7880. | 2.5 | 4 |
| 18 | Pragmatic Many-Body Approach for Economic MP2 Energy Estimation of Molecular Clusters. Journal of Physical Chemistry A, 2019, 123, 5005-5011. | 2.5 | 11 |

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| 19 | Preface. Journal of Computational Chemistry, 2018, 39, 457-457. | 3.3 | 0 |
| 20 | PAREMD: A parallel program for the evaluation of momentum space properties of atoms and molecules. Computer Physics Communications, 2018, 224, 299-310. | 7.5 | 13 |
| 21 | Electrostatics for probing lone pairs and their interactions. Journal of Computational Chemistry, 2018, 39, 488-499. | 3.3 | 37 |
| 22 | Harmonizing accuracy and efficiency: A pragmatic approach to fragmentation of large molecules. Journal of Chemical Physics, 2018, 149, 064112. | 3.0 | 15 |
| 23 | A Critical Analysis of the â€˜UGC-Approved List of Journalsâ€™. Current Science, 2018, 114, 1299. | 0.8 | 28 |
| 24 | Topology of molecular electron density and electrostatic potential with DAMQT. Computer Physics Communications, 2017, 214, 207-215. | 7.5 | 25 |
| 25 | Explicit hydration of ammonium ion by correlated methods employing molecular tailoring approach. Molecular Physics, 2017, 115, 2708-2720. | 1.7 | 7 |
| 26 | A combined theoretical and experimental study of phenol-(acetylene)n (n â‰¤ 7) clusters. Journal of Chemical Physics, 2017, 146, 154303. | 3.0 | 6 |
| 27 | Molecular Electrostatic Potential-Based Atoms in Molecules: Shielding Effects and Reactivity Patterns. Australian Journal of Chemistry, 2016, 69, 975. | 0.9 | 7 |
| 28 | Vibrational infrared and Raman spectra of polypeptides: Fragments-in-fragments within molecular tailoring approach. Journal of Chemical Physics, 2016, 144, 114113. | 3.0 | 32 |
| 29 | Breaking the bottleneck: Use of molecular tailoring approach for the estimation of binding energies at MP2/CBS limit for large water clusters. Journal of Chemical Physics, 2016, 144, 104102. | 3.0 | 20 |
| 30 | Bonding and Reactivity Patterns from Electrostatic Landscapes of Molecules. Journal of Chemical Sciences, 2016, 128, 1519-1526. | 1.5 | 9 |
| 31 | Toward an Accurate and Inexpensive Estimation of CCSD(T)/CBS Binding Energies of Large Water Clusters. Journal of Physical Chemistry A, 2016, 120, 5706-5714. | 2.5 | 31 |
| 32 | Exploring the Gradient Paths and Zero Flux Surfaces of Molecular Electrostatic Potential. Journal of Chemical Theory and Computation, 2016, 12, 1705-1713. | 5.3 | 17 |
| 33 | DAMQT 2.1.0: A new version of the DAMQT package enabled with the topographical analysis of electron density and electrostatic potential in molecules. Journal of Computational Chemistry, 2015, 36, 2350-2359. | 3.3 | 47 |
| 34 | Understanding Packing Patterns in Crystals by Analysis of Small Aggregates: A Case Study of CS<sub>2</sub>. Journal of Physical Chemistry A, 2015, 119, 13055-13063. | 2.5 | 7 |
| 35 | Hybrid QTAIM and electrostatic potential-based quantum topology phase diagrams for water clusters. Physical Chemistry Chemical Physics, 2015, 17, 15258-15273. | 2.8 | 9 |
| 36 | On the electrostatic nature of electrides. Physical Chemistry Chemical Physics, 2015, 17, 15030-15035. | 2.8 | 15 |

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| 37 | Stability of conformationally locked free fructose: theoretical and computational insights. New Journal of Chemistry, 2015, 39, 9006-9018. | 2.8 | 6 |
| 38 | Accurate vibrational spectra via molecular tailoring approach: A case study of water clusters at MP2 level. Journal of Chemical Physics, 2015, 142, 014107. | 3.0 | 20 |
| 39 | Structures, energetics and vibrational spectra of (H<sub>2</sub>O)<sub>32</sub>clusters: a journey from model potentials to correlated theory. Molecular Physics, 2015, 113, 2970-2979. | 1.7 | 18 |
| 40 | Low energy isomers of (H2O)25 from a hierarchical method based on Monte Carlo temperature basin paving and molecular tailoring approaches benchmarked by MP2 calculations. Journal of Chemical Physics, 2014, 141, 164304. | 3.0 | 23 |
| 41 | Molecular Tailoring Approach: A Route for ab Initio Treatment of Large Clusters. Accounts of Chemical Research, 2014, 47, 2739-2747. | 15.6 | 103 |
| 42 | Lone Pairs: An Electrostatic Viewpoint. Journal of Physical Chemistry A, 2014, 118, 526-532. | 2.5 | 89 |
| 43 | Quantum Chemical Investigations on Molecular Clusters. Chemical Reviews, 2014, 114, 12132-12173. | 47.7 | 170 |
| 44 | Molecular electrostatics for probing lone pairâ€“Ï€ interactions. Physical Chemistry Chemical Physics, 2013, 15, 18401. | 2.8 | 94 |
| 45 | High-Level ab Initio Investigations on Structures and Energetics of N<sub>2</sub>O Clusters. Journal of Physical Chemistry A, 2013, 117, 8591-8598. | 2.5 | 10 |
| 46 | Exploring Structures and Energetics of Large OCS Clusters by Correlated Methods. Journal of Physical Chemistry A, 2013, 117, 10964-10972. | 2.5 | 11 |
| 47 | Appraisal of molecular tailoring approach for large clusters. Journal of Chemical Physics, 2013, 138, 104101. | 3.0 | 54 |
| 48 | Studies toward Oxyacetamide-Linked RNA Analogues: Synthesis and Conformation of a Modified Dinucleoside. Synthesis, 2012, 44, 2277-2286. | 2.3 | 1 |
| 49 | Rapid topography mapping of scalar fields: Large molecular clusters. Journal of Chemical Physics, 2012, 137, 074116. | 3.0 | 21 |
| 50 | Facilitating Minima Search for Large Water Clusters at the MP2 Level via Molecular Tailoring. Journal of Physical Chemistry Letters, 2012, 3, 2253-2258. | 4.6 | 69 |
| 51 | Hydrogen Bond Energies and Cooperativity in Substituted Calix[n]arenes (n = 4, 5). Journal of Physical Chemistry A, 2012, 116, 3739-3744. | 2.5 | 37 |
| 52 | Structures, energetics and vibrational spectra of CO2 clusters through molecular tailoring and cluster building algorithm. Physical Chemistry Chemical Physics, 2012, 14, 7718. | 2.8 | 21 |
| 53 | Tailoring approach for obtaining molecular orbitals of large systems#. Journal of Chemical Sciences, 2012, 124, 149-158. | 1.5 | 7 |
| 54 | Acetylene aggregates via cluster-building algorithm and molecular tailoring approach. Theoretical Chemistry Accounts, 2012, 131, 1. | 1.4 | 16 |

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| 55 | Topography of Scalar Fields: Molecular Clusters and Ï€-Conjugated Systems. Journal of Physical Chemistry A, 2011, 115, 12769-12779. | 2.5 | 23 |
| 56 | â€œGold standardâ€•coupled-cluster study of acetylene pentamers and hexamers via molecular tailoring approach. Theoretical Chemistry Accounts, 2011, 130, 491-500. | 1.4 | 28 |
| 57 | Intramolecular hydrogen bond energy and cooperative interactions in Î±â€, Î²â€, and Î³â€cyclodextrin conformers. Journal of Computational Chemistry, 2011, 32, 2996-3004. | 3.3 | 46 |
| 58 | Molecular cluster building algorithm: Electrostatic guidelines and molecular tailoring approach. Journal of Chemical Physics, 2011, 134, 084111. | 3.0 | 45 |
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| 61 | On the applicability of fragmentation methods to conjugated Ï€ systems within density functional framework. Journal of Chemical Physics, 2010, 132, 094102. | 3.0 | 55 |
| 62 | Ab initioinvestigation of benzene clusters: Molecular tailoring approach. Journal of Chemical Physics, 2010, 133, 164308. | 3.0 | 73 |
| 63 | Appraisal of Through-Bond and Through-Space Substituent Effects via Molecular Electrostatic Potential Topography. Journal of Physical Chemistry A, 2010, 114, 12330-12333. | 2.5 | 35 |
| 64 | WebMTA: A webâ€interface for ab initio geometry optimization of large molecules using molecular tailoring approach. Journal of Computational Chemistry, 2009, 30, 1167-1173. | 3.3 | 15 |
| 65 | Signatures of molecular recognition from the topography of electrostatic potential. Journal of Chemical Sciences, 2009, 121, 815-821. | 1.5 | 26 |
| 66 | Ab initio study on (CO<sub>2</sub>)<sub>n</sub>clusters via electrostaticsâ€•and molecular tailoringâ€based algorithm. International Journal of Quantum Chemistry, 2009, 109, 2238-2247. | 2.0 | 19 |
| 67 | Significant progress in predicting the crystal structures of small organic molecules â€“ a report on the fourth blind test. Acta Crystallographica Section B: Structural Science, 2009, 65, 107-125. | 1.8 | 371 |
| 68 | Stepwise Hydration of Protonated Carbonic Acid: A Theoretical Study. Journal of Physical Chemistry A, 2009, 113, 12260-12275. | 2.5 | 27 |
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| 72 | Quantum chemical and electrostatic studies of anionic water clusters, <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" altimg="si17.gif" overflow="scroll"><mml:mrow><mml:mmultiscripts><mml:mrow><mml:msub><mml:mrow><mml:mtext>(H</mml:mtext></mml:mrow /><mml:none /><mml:mrow><mml:mo>-</mml:mo></mml:mrow></mml:msub></mml:mrow></mml:mmultiscripts></mml:mrow></mml:math>. Computational and Theoretical Chemistry, 2008, 851, 213-219. | 1.5 | 10 |

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| 73 | Cation-Ï€ interaction: to stack or to spread. Molecular Physics, 2008, 106, 1557-1566. | 1.7 | 19 |
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| 76 | Structure, Energetics, and Reactivity of Boric Acid Nanotubes: A Molecular Tailoring Approach. Journal of Physical Chemistry A, 2008, 112, 7699-7704. | 2.5 | 36 |
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| 81 | Electrostatic guidelines and molecular tailoring for density functional investigation of structures and energetics of (Li)n clusters. Journal of Chemical Physics, 2008, 129, 164314. | 3.0 | 23 |
| 82 | Intramolecular Hydrogen Bond Energy in Polyhydroxy Systems:â€‰ A Critical Comparison of Molecular Tailoring and Isodesmic Approaches. Journal of Physical Chemistry A, 2007, 111, 6472-6480. | 2.5 | 67 |
| 83 | Electrostatic Potential Minimum of the Aromatic Ring as a Measure of Substituent Constant. Journal of Physical Chemistry A, 2007, 111, 710-714. | 2.5 | 91 |
| 84 | Effect of matrix on IR frequencies of acetylene and acetylene-methanol complex: Infrared matrix isolation and ab initio study. Journal of Chemical Physics, 2007, 127, 104501. | 3.0 | 46 |
| 85 | Electrostatic Potential Topography for Exploring Electronic Reorganizations in 1,3 Dipolar Cycloadditions. Journal of Physical Chemistry A, 2007, 111, 2733-2738. | 2.5 | 28 |
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| 87 | Can Ring Strain Be Realized in Momentum Space?. Journal of the American Chemical Society, 2006, 128, 10702-10706. | 13.7 | 8 |
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| 89 | Molecular tailoring approach for geometry optimization of large molecules: Energy evaluation and parallelization strategies. Journal of Chemical Physics, 2006, 125, 104109. | 3.0 | 246 |
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| 91 | Adsorption of water on sodium chloride surfaces: electrostatics â€“ guided ab initio studies. Theoretical Chemistry Accounts, 2005, 114, 129-136. | 1.4 | 9 |
| 92 | Topography of molecular scalar fields. II. An appraisal of the hierarchy principle for electron momentum densities. Journal of Chemical Physics, 2005, 122, 164108. | 3.0 | 2 |
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| 96 | Tailoring approach for exploring electron densities and electrostatic potentials of molecular crystals. Theoretical Chemistry Accounts, 2004, 111, 255-263. | 1.4 | 71 |
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| 99 | Structure, Reactivity and Aromaticity of Acenes and Their BN Analogues: A Density Functional and Electrostatic Investigation. Inorganic Chemistry, 2004, 43, 5824-5832. | 4.0 | 61 |
| 100 | Ab initio quality one-electron properties of large molecules: Development and testing of molecular tailoring approach. Journal of Computational Chemistry, 2003, 24, 484-495. | 3.3 | 133 |
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| 103 | Hâ‹Ï€ Complexes of Acetyleneâ‹Ethylene:â€‰ A Matrix Isolation and Computational Study. Journal of Physical Chemistry A, 2002, 106, 1504-1510. | 2.5 | 85 |
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| 107 | Hâ‹Ï€ complexes of acetyleneâ€“benzene: a matrix isolation and computational study. Journal of Molecular Structure, 2002, 613, 209-222. | 3.6 | 63 |
| 108 | Revisiting Markovnikov Addition to Alkenes via Molecular Electrostatic Potential. Journal of Organic Chemistry, 2001, 66, 6883-6890. | 3.2 | 66 |

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| 109 | Structure and Stability of Water Clusters (H2O)n, n = 8â^'20:â€‰ An Ab Initio Investigation. Journal of Physical Chemistry A, 2001, 105, 10525-10537. | 2.5 | 459 |
| 110 | Century of Nobel Prizes. Resonance, 2001, 6, 36-43. | 0.3 | 3 |
| 111 | Theoretical investigations on structure, electrostatic potentials and vibrational frequencies of diglyme and Li+â€"(diglyme) conformers. Chemical Physics Letters, 2001, 344, 527-535. | 2.6 | 16 |
| 112 | Polarization-corrected molecular electrostatic potential for the cation binding problem. Chemical Physics Letters, 2001, 340, 604-610. | 2.6 | 5 |
| 113 | Molecular Electrostatic Potential and Electron Density Topography:â€‰ Structure and Reactivity of (substituted arene)Cr(CO)3 Complexes. Organometallics, 2000, 19, 3008-3015. | 2.3 | 63 |
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| 115 | Does a Stacked DNA Base Pair Hydrate Better than a Hydrogen-Bonded One?:Â An ab Initio Study. Journal of Physical Chemistry A, 2000, 104, 10887-10894. | 2.5 | 53 |
| 116 | Topography of Atomic and Molecular Scalar Fields. Computational Chemistry - Reviews of Current Trends, 1999, , 1-53. | 0.4 | 7 |
| 117 | Ab Initio Structure and Vibrational Frequencies of (CF3SO2)2N-Li+Ion Pairs. Journal of Physical Chemistry A, 1999, 103, 7474-7480. | 2.5 | 110 |
| 118 | Electrostatics in chemistry. Resonance, 1999, 4, 11-20. | 0.3 | 4 |
| 119 | Electrostatics in chemistry. Resonance, 1999, 4, 8-19. | 0.3 | 4 |
| 120 | Electrostatics in chemistry. Resonance, 1999, 4, 14-23. | 0.3 | 3 |
| 121 | Electrostatics in chemistry. Resonance, 1999, 4, 40-51. | 0.3 | 0 |
| 122 | Clar's Aromatic Sextet Theory Revisited via Molecular Electrostatic Potential Topography. Journal of Organic Chemistry, 1999, 64, 2505-2512. | 3.2 | 127 |
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| 124 | Complexes of ammonia with propane and cyclopropane: electrostatic guidelines for ab initio treatment. Theoretical Chemistry Accounts, 1998, 100, 300-306. | 1.4 | 6 |
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| 126 | A Novel Electrostatic Approach to Substituent Constants:Â Doubly Substituted Benzenes. Journal of the American Chemical Society, 1998, 120, 7049-7055. | 13.7 | 95 |

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| 127 | Polarization-Corrected Electrostatic Potential for Probing Cation Binding Patterns of Molecules. 1. Saturated Hydrocarbons. Journal of the American Chemical Society, 1998, 120, 7056-7062. | 13.7 | 24 |
| 128 | Electrostatic Insights into the Molecular Hydration Process: A Case Study of Crown Ethersâ€. Journal of Physical Chemistry A, 1998, 102, 9987-9992. | 2.5 | 57 |
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| 131 | Electronic Perturbations of the Aromatic Nucleus:Â Hammett Constants and Electrostatic Potential Topographyâ€. Journal of Organic Chemistry, 1997, 62, 2625-2627. | 3.2 | 82 |
| 132 | Electrostatic Potential as a Harbinger of Cation Coordination:Â CF3SO3-Ion as a Model Example. Journal of Physical Chemistry A, 1997, 101, 5678-5686. | 2.5 | 37 |
| 133 | Structure and Stability of DNA Base Trimers:Â An Electrostatic Approach. Journal of Physical Chemistry B, 1997, 101, 9657-9662. | 2.6 | 54 |
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| 139 | Basis set dependence of the molecular electrostatic potential topography. A case study of substituted benzenes. Chemical Physics Letters, 1995, 239, 273-281. | 2.6 | 60 |
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| 141 | Topographical Analysis of Electron Density and Molecular Electrostatic Potential for Cyclopropa- and Cyclobutabenzenes. Journal of the American Chemical Society, 1995, 117, 9559-9563. | 13.7 | 21 |
| 142 | Molecular Tailoring Approach for Simulation of Electrostatic Properties. The Journal of Physical Chemistry, 1994, 98, 9165-9169. | 2.9 | 173 |
| 143 | Closo-Boranes, -Carboranes, and -Silaboranes: A Topographical Study Using Electron Density and Molecular Electrostatic Potential. The Journal of Physical Chemistry, 1994, 98, 6445-6451. | 2.9 | 25 |
| 144 | Molecular electrostatic charge models: A topographical approach. International Journal of Quantum Chemistry, 1994, 49, 397-407. | 2.0 | 7 |

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| 145 | Comment on â€œComputing molecular electrostatic potentials with the PRISM algorithmâ€• Chemical Physics Letters, 1994, 218, 593-594. | 2.6 | 1 |
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| 152 | Development of a restricted Hartree?Fock program INDMOL on PARAM: A highly parallel computer. Journal of Computational Chemistry, 1993, 14, 445-451. | 3.3 | 31 |
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