Steven Robert Kirk

List of Publications by Year
in descending order

108	1,965	236925 25	345221 36
papers	citations	h-index	g-index

110	110	110	1486
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	Software architecture graphs as complex networks: A novel partitioning scheme to measure stability and evolution. Information Sciences, 2007, 177, 2587-2601.	6.9	85
2	Bamboo-derived porous biochar for efficient adsorption removal of dibenzothiophene from model fuel. Fuel, 2018, 211, 121-129.	6.4	73
3	The response of the electronic structure to electronic excitation and double bond torsion in fulvene: a combined QTAIM, stress tensor and MO perspective. Physical Chemistry Chemical Physics, 2014, 16, 7115-7126.	2.8	58
4	Pointing the way to the products? Comparison of the stress tensor and the second-derivative tensor of the electron density. Journal of Chemical Physics, 2011, 134, 234106.	3.0	52
5	Bond metallicity of materials from real space charge density distributions. Chemical Physics Letters, 2009, 471, 174-177.	2.6	51
6	Spanning QTAIM topology phase diagrams of water isomers W4, W5 and W6. Physical Chemistry Chemical Physics, 2011, 13, 11644.	2.8	48
7	Ï€â€Extended â€œEarringâ€•Porphyrins with Multiple Cavities and Nearâ€Infrared Absorption. Angewandte Chemie - International Edition, 2016, 55, 6438-6442.	13.8	47
8	Biphenyl: A stress tensor and vector-based perspective explored within the quantum theory of atoms in molecules. International Journal of Quantum Chemistry, 2015, 115, 1678-1690.	2.0	46
9	Solvent-free selective oxidation of toluene by oxygen over MnOx/SBA-15 catalysts: Relationship between catalytic behavior and surface structure. Chemical Engineering Journal, 2015, 280, 737-747.	12.7	46
10	Dependence of the normal modes on the electronic structure of various phases of ice as calculated by ab initio methods. Canadian Journal of Physics, 2003, 81, 225-231.	1.1	42
11	The Ehrenfest force topology: a physically intuitive approach for analyzing chemical interactions. Physical Chemistry Chemical Physics, 2013, 15, 17823.	2.8	38
12	Distinguishing and quantifying the torquoselectivity in competitive ring-opening reactions using the stress tensor and QTAIM. Journal of Computational Chemistry, 2016, 37, 2722-2733.	3.3	38
13	Visible light-triggered vanadium-substituted molybdophosphoric acids to catalyze liquid phase oxygenation of cyclohexane to KA oil by nitrous oxide. Applied Catalysis B: Environmental, 2016, 182, 392-404.	20.2	37
14	Biochar sulfonic acid immobilized chlorozincate ionic liquid: an efficiently biomimetic and reusable catalyst for hydrolysis of cellulose and bamboo under microwave irradiation. Cellulose, 2014, 21, 1227-1237.	4.9	36
15	A non-nitric acid method of adipic acid synthesis: organic solvent- and promoter-free oxidation of cyclohexanone with oxygen over hollow-structured Mn/TS-1 catalysts. Green Chemistry, 2015, 17, 1884-1892.	9.0	36
16	Oxidation of cyclohexane to adipic acid catalyzed by Mn-doped titanosilicate with hollow structure. Catalysis Communications, 2015, 58, 46-52.	3.3	36
17	Structures, energies and bonding in neutral and charged Li microclusters. Journal of Molecular Modeling, 2012, 18, 4171-4189.	1.8	35
18	Effective transformation of cellulose to 5-hydroxymethylfurfural catalyzed by fluorine anion-containing ionic liquid modified biochar sulfonic acids in water. Cellulose, 2017, 24, 95-106.	4.9	35

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19	The mechanics of charge-shift bonds: A perspective from the electronic stress tensor. Chemical Physics Letters, 2011, 510, 18-20.	2.6	31
20	Molecular dynamics simulation of nanocolloidal amorphous silica particles: Part I. Journal of Chemical Physics, 2007, 127, 224711.	3.0	29
21	A stress tensor eigenvector projection space for the (H2O)5 potential energy surface. Chemical Physics Letters, 2017, 667, 25-31.	2.6	29
22	Chiralityâ€“Helicity Equivalence in the S and R Stereoisomers: AÂTheoretical Insight. Journal of the American Chemical Society, 2019, 141, 5497-5503.	13.7	29
23	Spanning Set of Silica Cluster Isomer Topologies from QTAIM. Journal of Physical Chemistry A, 2011, 115, 12503-12511.	2.5	28
24	Synergistic hydrogen atom transfer with the active role of solvent: Preferred one-step aerobic oxidation of cyclohexane to adipic acid by N-hydroxyphthalimide. Journal of Catalysis, 2019, 378, 256-269.	6.2	28
25	Information theory-based software metrics and obfuscation. Journal of Systems and Software, 2004, 72, 179-186.	4.5	26
26	Exploring hydrogen bond in the excited state leading toward intramolecular proton transfer: detailed analysis of the structure and charge density topology along the reaction path using QTAIM. Journal of Molecular Modeling, 2012, 18, 4225-4237.	1.8	26
27	Vanadiumâ€Substituted Tungstophosphoric Acids as Efficient Catalysts for Visibleâ€Lightâ€Driven Oxygenation of Cyclohexane by Dioxygen. ChemCatChem, 2015, 7, 2637-2645.	3.7	26
28	Origin of the cis-Effect: a Density Functional Theory Study of Doubly Substituted Ethylenes. Wuli Huaxue Xuebao/ Acta Physico - Chimica Sinica, 2013, 29, 43-54.	4.9	25
29	Non-nuclear attractors in small charged lithium clusters, Li_m^q (m =) Tj ETQq1 1 0.784314 rgBT /Ove Physics, 2018, 20, 24695-24707.	2.8	24
30	Fatigue and photochromism S₁ excited state reactivity of diarylethenes from QTAIM and the stress tensor. International Journal of Quantum Chemistry, 2018, 118, e25565.	2.0	23
31	Stress tensor eigenvector following with nextâ€generation quantum theory of atoms in molecules. International Journal of Quantum Chemistry, 2019, 119, e25847.	2.0	23
32	Light-triggered oxy-chlorination of cyclohexane by metal chlorides. Applied Catalysis A: General, 2014, 469, 483-489.	4.3	21
33	Quinoneâ€based switches for candidate building blocks of molecular junctions with QTAIM and the stress tensor. International Journal of Quantum Chemistry, 2018, 118, e25676.	2.0	21
34	Molecular dynamics simulation of nanocolloidal amorphous silica particles: Part II. Journal of Chemical Physics, 2008, 128, 164711.	3.0	20
35	Azobenzeneâ€Bridged Porphyrin Nanorings: Syntheses, Structures, and Photophysical Properties. Chemistry - A European Journal, 2015, 21, 15328-15338.	3.3	20
36	The normal modes of vibration of benzene from the trajectories of stress tensor eigenvector projection space. Chemical Physics Letters, 2017, 677, 156-161.	2.6	20

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37	11-cis retinal torsion: A QTAIM and stress tensor analysis of the S1 excited state. Chemical Physics Letters, 2016, 652, 112-116.	2.6	19
38	QTAIM and stress tensor bond-path framework sets for the ground and excited states of fulvene. Chemical Physics Letters, 2018, 713, 125-131.	2.6	19
39	Intramolecular mode coupling of the isotopomers of water: a non-scalar charge density-derived perspective. Physical Chemistry Chemical Physics, 2020, 22, 2509-2520.	2.8	19
40	Nextâ€generation quantum theory of atoms in molecules for the ground and excited states of fulvene. International Journal of Quantum Chemistry, 2018, 118, e25768.	2.0	18
41	Nextâ€generation quantum theory of atoms in molecules for the ground and excited state of the ringâ€opening of cyclohexadiene. International Journal of Quantum Chemistry, 2019, 119, e25862.	2.0	18
42	A bond, ring and cage resolved PoincarÃ©â€“Hopf relationship for isomerisation reaction pathways. Molecular Physics, 2013, 111, 3104-3116.	1.7	17
43	QTAIM and Stress Tensor Characterization of Intramolecular Interactions Along Dynamics Trajectories of a Light-Driven Rotary Molecular Motor. Journal of Physical Chemistry A, 2017, 121, 4778-4792.	2.5	17
44	3-D bond-paths of QTAIM and the stress tensor in neutral lithium clusters, Li_m (m =) Tj ETQq0 0 0 rgBT /Overlock 10 22, 864-877.	2.8	16
45	Chlorocuprate Ionic Liquid Functionalized Biochar Sulfonic Acid as an Efficiently Biomimetic Catalyst for Direct Hydrolysis of Bamboo under Microwave Irradiation. Industrial & Engineering Chemistry Research, 2013, 52, 11537-11543.	3.7	15
46	A QTAIM and stress tensor investigation of the torsion path of a light-driven fluorene molecular rotary motor. Journal of Computational Chemistry, 2016, 37, 2588-2596.	3.3	15
47	The directional bonding of [1.1.1]propellane with next generation QTAIM. Chemical Physics Letters, 2019, 730, 506-512.	2.6	15
48	The destabilization of hydrogen bonds in an external Eâ€field for improved switch performance. Journal of Computational Chemistry, 2019, 40, 1881-1891.	3.3	15
49	The cis-effect using the topology of the electronic charge density. Molecular Physics, 2013, 111, 793-805.	1.7	14
50	Next-generation quantum theory of atoms in molecules for the ground and excited state of DHCL. Chemical Physics Letters, 2019, 717, 91-98.	2.6	14
51	Preparation of Fe2O3 doped SBA-15 for vapor phase ortho-position C-alkylation of phenol with methanol. Catalysis Communications, 2017, 92, 90-94.	3.3	13
52	Exploration of the forbidden regions of the Ramachandran plot (Ï•-Ï) with QTAIM. Physical Chemistry Chemical Physics, 2017, 19, 26423-26434.	2.8	13
53	The role of hydrogen bonding in nanocolloidal amorphous silica particles in electrolyte solutions. Journal of Colloid and Interface Science, 2009, 339, 351-361.	9.4	12
54	Tiling for Performance Tuning on Different Models of GPUs. , 2009, , .		12

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55	Nextâ€generation quantum theory of atoms in molecules for the photochemical ringâ€opening reactions of oxirane. International Journal of Quantum Chemistry, 2019, 119, e25957.	2.0	12
56	Nextâ€generation quantum theory of atoms in molecules for the S₁/S₀ conical intersections in dynamics trajectories of a lightâ€driven rotary molecular motor. International Journal of Quantum Chemistry, 2020, 120, e26062.	2.0	12
57	Nextâ€generation QTAIM for scoring molecular wires in Eâ€fields for molecular electronic devices. Journal of Computational Chemistry, 2020, 41, 913-921.	3.3	12
58	A comparison of QTAIM and the stress tensor for Chirality-Helicity equivalence in S and R stereoisomers. Chemical Physics Letters, 2020, 738, 136907.	2.6	12
59	Molecular dynamics simulation of nanocolloidal amorphous silica particles: Part III. Journal of Chemical Physics, 2009, 130, 134702.	3.0	11
60	The Pt site reactivity of the molecular graphs of Au6Pt isomers. Chemical Physics Letters, 2013, 590, 41-45.	2.6	11
61	Direct cyclohexanone oxime synthesis via oxidationâ€“oximization of cyclohexane with ammonium acetate. Chemical Communications, 2020, 56, 1436-1439.	4.1	11
62	Electronic Stress as a Guiding Force for Chemical Bonding. Topics in Current Chemistry, 2011, 351, 103-124.	4.0	10
63	New non-metallic mesoporous SBA-15 catalyst with high selectivity for the gas-phase oxidation of cyclohexylamine to cyclohexanone oxime. Catalysis Communications, 2014, 56, 148-152.	3.3	10
64	Quantum topology phase diagrams for the cisâ€and transâ€isomers of the cyclic contryphanâ€6m peptide. International Journal of Quantum Chemistry, 2014, 114, 1697-1706.	2.0	10
65	The substituent effects on the biphenyl Hâ‹¯H bonding interactions subjected to torsion. Chemical Physics Letters, 2016, 651, 251-256.	2.6	10
66	QTAIM and stress tensor interpretation of the (H₂ O)₅ potential energy surface. Journal of Computational Chemistry, 2016, 37, 2712-2721.	3.3	10
67	A QTAIM exploration of the competition between hydrogen and halogen bonding in halogenated 1-methyluracil: Water systems. Chemical Physics Letters, 2016, 662, 67-72.	2.6	10
68	Stress Tensor Eigenvector Following with Next-Generation Quantum Theory of Atoms in Molecules: Excited State Photochemical Reaction Path from Benzene to Benzvalene. Journal of Physical Chemistry A, 2019, 123, 8254-8264.	2.5	10
69	Beyond energetic and scalar measures: Next generation <scp>quantum theory of atoms in molecules</scp>. Wiley Interdisciplinary Reviews: Computational Molecular Science, 2022, 12, .	14.6	10
70	Hybrid QTAIM and electrostatic potential-based quantum topology phase diagrams for water clusters. Physical Chemistry Chemical Physics, 2015, 17, 15258-15273.	2.8	9
71	The 3-D bonding morphology of the infra-red active normal modes of benzene. Chemical Physics Letters, 2018, 710, 31-38.	2.6	9
72	A 3â€D bonding perspective of the factors influencing the relative stability of the S1/S0conical intersections of the pentaâ€2,4â€dieniminium cation (PSB3). International Journal of Quantum Chemistry, 2019, 119, e25903.	2.0	9

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73	Next generation QTAIM for the design of quinone-based switches. Chemical Physics Letters, 2019, 722, 110-118.	2.6	9
74	Chiralityâ€"helicity of cumulenes: A nonâ€scalar charge density derived perspective. International Journal of Quantum Chemistry, 2022, 122, .	2.0	9
75	Allylic oxidation of Î±-isophorone to keto-isophorone with molecular oxygen catalyzed by copper chloride in acetylacetone. Applied Catalysis A: General, 2014, 486, 193-200.	4.3	8
76	Consideration of roles of commercial TiO2 pigments in aromatic polyurethane coating via the photodegradation of dimethyl toluene-2,4-dicarbamate in non-aqueous solution. Research on Chemical Intermediates, 2015, 41, 7785-7797.	2.7	8
77	A QTAIM and stress tensor perspective of large-amplitude motions of the tetrasulfur tetranitride S₄N₄molecular graph. International Journal of Quantum Chemistry, 2016, 116, 1025-1039.	2.0	8
78	Insights into the all-metal [Sb3Au3Sb3]3â^' sandwich complex from a QTAIM and stress tensor analysis. Chemical Physics Letters, 2017, 685, 127-132.	2.6	8
79	Halogen and Hydrogen Bonding in Halogenabenzene/NH3 Complexes Compared Using Next-Generation QTAIM. Molecules, 2019, 24, 2875.	3.8	8
80	Fatigue and fatigue resistance in S 1 excited state diarylethenes in electric fields. International Journal of Quantum Chemistry, 2021, 121, e26527.	2.0	8
81	Control of chirality, bond flexing and anharmonicity in an electric field. International Journal of Quantum Chemistry, 2021, 121, e26793.	2.0	8
82	Chirality without Stereoisomers: Insight fromÂthe Helical Response of Bond Electrons. ChemPhysChem, 2021, 22, 1989-1995.	2.1	8
83	Chiral and steric effects in ethane: A next generation QTAIM interpretation. Chemical Physics Letters, 2022, 800, 139669.	2.6	8
84	The role of weak interactions in characterizing peptide folding preferences using a QTAIM interpretation of the Ramachandran plot (Ï•â€Ï). International Journal of Quantum Chemistry, 2018, 118, e25456.	2.0	7
85	Explanation of the role of hydrogen bonding in the structural preferences of small molecule conformers. Chemical Physics Letters, 2019, 730, 206-212.	2.6	7
86	An explanation of the unusual strength of the <scp>hydrogen bond</scp> in small water clusters. International Journal of Quantum Chemistry, 2020, 120, e26361.	2.0	7
87	Mixed chiral and achiral character in substituted ethane: A next generation QTAIM perspective. Chemical Physics Letters, 2022, 803, 139762.	2.6	7
88	A vectorâ€based representation of the chemical bond for predicting competitive and noncompetitive torquoselectivity of thermal ringâ€opening reactions. International Journal of Quantum Chemistry, 2018, 118, e25707.	2.0	6
89	A vector-based representation of the chemical bond for the substituted torsion of biphenyl. Chemical Physics Letters, 2018, 702, 32-37.	2.6	6
90	Imidazolyl activated carbon refluxed with ethanediamine as reusable heterogeneous catalysts for Michael addition. RSC Advances, 2019, 9, 185-191.	3.6	6

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91	Flip rearrangement in the water pentamer: Analysis of electronic structure. International Journal of Quantum Chemistry, 2020, 120, e26124.	2.0	6
92	Photochemical ring-opening reactions of oxirane with the Ehrenfest force topology. Chemical Physics Letters, 2021, 769, 138432.	2.6	6
93	Molecular dynamics simulations of the aggregation of nanocolloidal amorphous silica monomers and dimers. Procedia Engineering, 2011, 18, 188-193.	1.2	5
94	A QTAIM perspective of the Si6Li6 potential energy surface using quantum topology phase diagrams. Chemical Physics Letters, 2014, 609, 117-122.	2.6	5
95	A vectorâ€based representation of the chemical bond for the normal modes of benzene. International Journal of Quantum Chemistry, 2018, 118, e25698.	2.0	5
96	The role of the natural transition orbital density in the S0Âât'ÂS1 and S0Âât'ÂS2 transitions of fulvene with next generation QTAIM. Chemical Physics Letters, 2020, 751, 137556.	2.6	5
97	Bond-path-rigidity and bond-path-flexibility of the ground state and first excited state of fulvene. Chemical Physics Letters, 2021, 766, 138339.	2.6	5
98	Bond flexing, twisting, anharmonicity and responsivity for the infraredâ€active modes of benzene. International Journal of Quantum Chemistry, 2021, 121, e26584.	2.0	5
99	Hydroxyl-assisted selective epoxidation of perillyl alcohol with hydrogen peroxide by vanadium-substituted phosphotungstic acid hinged on imidazolyl activated carbon. New Journal of Chemistry, 2022, 46, 6636-6645.	2.8	5
100	Highly efficient and recyclable alkylammonium hydrosulfate catalyst for formation of bisphenol F by condensation of phenol with formaldehyde. RSC Advances, 2016, 6, 92716-92722.	3.6	4
101	Next generation quantum theory of atoms in molecules for the design of emitters exhibiting thermally activated delayed fluorescence with laser irradiation. Journal of Computational Chemistry, 2022, 43, 206-214.	3.3	4
102	Quantum topological resolution of catalyst proficiency. International Journal of Quantum Chemistry, 2015, 115, 875-883.	2.0	3
103	Isomerization of the RPSB chromophore in the gas phase along the torsional pathways using QTAIM. Chemical Physics Letters, 2017, 685, 222-228.	2.6	3
104	Understanding chemical coupling in cyclic versus compact water clusters with the Ehrenfest Force. Chemical Physics Letters, 2021, 781, 138983.	2.6	3
105	The chirality of isotopomers of glycine compared using nextâ€generation <scp>QTAIM</scp>. International Journal of Quantum Chemistry, 0, , .	2.0	3
106	Selective Catalytic Isomerization of Î²â€Pinene Oxide to Perillyl Alcohol Enhanced by Protic Tetraimidazolium Nitrate. ChemistryOpen, 2021, 10, 477-485.	1.9	2
107	Consequences of theory level choice evaluated with new tools from QTAIM and the stress tensor for a dipeptide conformer. Chemical Physics Letters, 2018, 696, 42-47.	2.6	1
108	Nano-Silica@PVC-Bonded N-Ethyl Sulfamic Acid as a Recyclable Solid Catalyst for the Hydroxyalkylation of Phenol with Formaldehyde to Bisphenol F. Bulletin of the Chemical Society of Japan, 2019, 92, 1394-1403.	3.2	1