Yunwen Tao

List of Publications by Year
in descending order

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103	4,704	147801	106344
papers	citations	31 h-index	65 g-index

106	106	106	3248
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	Chemical Bonds without Bonding Electron Density ? Does the Difference Electron-Density Analysis Suffice for a Description of the Chemical Bond?. Angewandte Chemie International Edition in English, 1984, 23, 627-628.	4.4	1,276
2	Computational Analysis of the Mechanism of Chemical Reactions in Terms of Reaction Phases: Hidden Intermediates and Hidden Transition States. Accounts of Chemical Research, 2010, 43, 591-601.	15.6	160
3	Machine learning of serum metabolic patterns encodes early-stage lung adenocarcinoma. Nature Communications, 2020, 11, 3556.	12.8	151
4	Identification of the Strongest Bonds in Chemistry. Journal of Physical Chemistry A, 2013, 117, 8981-8995.	2.5	140
5	Strength of the Pnicogen Bond in Complexes Involving Group Va Elements N, P, and As. Journal of Physical Chemistry A, 2015, 119, 1642-1656.	2.5	132
6	The intrinsic strength of the halogen bond: electrostatic and covalent contributions described by coupled cluster theory. Physical Chemistry Chemical Physics, 2016, 18, 33031-33046.	2.8	128
7	A comprehensive analysis of hydrogen bond interactions based on local vibrational modes. International Journal of Quantum Chemistry, 2012, 112, 3174-3187.	2.0	121
8	Relating normal vibrational modes to local vibrational modes with the help of an adiabatic connection scheme. Journal of Chemical Physics, 2012, 137, 084114.	3.0	113
9	The Many Facets of Chalcogen Bonding: Described by Vibrational Spectroscopy. Journal of Physical Chemistry A, 2017, 121, 6845-6862.	2.5	95
10	Quantitative Assessment of Halogen Bonding Utilizing Vibrational Spectroscopy. Inorganic Chemistry, 2017, 56, 488-502.	4.0	91
11	Reâ€evaluation of the bond lengthâ€“bond strength rule: The stronger bond is not always the shorter bond. Journal of Computational Chemistry, 2016, 37, 130-142.	3.3	88
12	Direct Measure of Metalâ€“Ligand Bonding Replacing the Tolman Electronic Parameter. Inorganic Chemistry, 2016, 55, 2332-2344.	4.0	85
13	Different Ways of Hydrogen Bonding in Water - Why Does Warm Water Freeze Faster than Cold Water?. Journal of Chemical Theory and Computation, 2017, 13, 55-76.	5.3	85
14	Decoding chemical information from vibrational spectroscopy data: Local vibrational mode theory. Wiley Interdisciplinary Reviews: Computational Molecular Science, 2020, 10, e1480.	14.6	85
15	Quantitative Assessment of Tetrel Bonding Utilizing Vibrational Spectroscopy. Molecules, 2018, 23, 2763.	3.8	84
16	Systematic Coupled Cluster Study of Noncovalent Interactions Involving Halogens, Chalcogens, and Pnicogens. Journal of Physical Chemistry A, 2017, 121, 9544-9556.	2.5	72
17	Strengthening of hydrogen bonding with the push-pull effect. Chemical Physics Letters, 2017, 685, 251-258.	2.6	58
18	Quantitative Assessment of Aromaticity and Antiaromaticity Utilizing Vibrational Spectroscopy. Journal of Organic Chemistry, 2016, 81, 9669-9686.	3.2	56

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19	Hidden Bond Anomalies: The Peculiar Case of the Fluorinated Amine Chalcogenides. Journal of Physical Chemistry A, 2015, 119, 9541-9556.	2.5	54
20	Reaction path Hamiltonian and the unified reaction valley approach. Wiley Interdisciplinary Reviews: Computational Molecular Science, 2011, 1, 531-556.	14.6	47
21	Chelation-Assisted Selective Etching Construction of Hierarchical Polyoxometalate-Based Metalâ€“Organic Framework. Chemistry of Materials, 2020, 32, 5550-5557.	6.7	43
22	Are carbonâ€”halogen double and triple bonds possible?. International Journal of Quantum Chemistry, 2014, 114, 1060-1072.	2.0	41
23	A New Method for Describing the Mechanism of a Chemical Reaction Based on the Unified Reaction Valley Approach. Journal of Chemical Theory and Computation, 2016, 12, 650-663.	5.3	41
24	Rational Design in Catalysis: A Mechanistic Study of Î²-Hydride Eliminations in Gold(I) and Gold(III) Complexes Based on Features of the Reaction Valley. Inorganic Chemistry, 2016, 55, 8636-8645.	4.0	40
25	Accurate determination of the binding energy of the formic acid dimer: The importance of geometry relaxation. Journal of Chemical Physics, 2014, 140, 084315.	3.0	39
26	A Continuum from Halogen Bonds to Covalent Bonds: Where Do Î»3 Iodanes Fit?. Inorganics, 2019, 7, 47.	2.7	39
27	Extraordinary Mechanism of the Dielsâ€“Alder Reaction: Investigation of Stereochemistry, Charge Transfer, Charge Polarization, and Biradicaloid Formation. Journal of Physical Chemistry A, 2016, 120, 1097-1111.	2.5	37
28	A Sodaliteâ€Type Silver Orthophosphate Cluster in a Globular Silver Nanocluster. Angewandte Chemie - International Edition, 2020, 59, 12659-12663.	13.8	36
29	New insights into Feâ€“H$$_{2}$$ and Feâ€“H$$^{-}$$ bonding of a [NiFe] hydrogenase mimic: a local vibrational mode study. Theoretical Chemistry Accounts, 2019, 138, 1.	1.4	34
30	A new way of studying chemical reactions: a hand-in-hand URVA and QTAIM approach. Physical Chemistry Chemical Physics, 2019, 21, 15007-15018.	2.8	33
31	Enediynes, enyneâ€allenes, their reactions, and beyond. Wiley Interdisciplinary Reviews: Computational Molecular Science, 2014, 4, 285-324.	14.6	32
32	Interplay of Ring Puckering and Hydrogen Bonding in Deoxyribonucleosides. Journal of Physical Chemistry A, 2019, 123, 7087-7103.	2.5	32
33	In Situ Measure of Intrinsic Bond Strength in Crystalline Structures: Local Vibrational Mode Theory for Periodic Systems. Journal of Chemical Theory and Computation, 2019, 15, 1761-1776.	5.3	32
34	Energetics and Mechanism of the Hydrogenation of XH_n for Group IV to Group VII Elements X. Journal of Chemical Theory and Computation, 2012, 8, 4931-4943.	5.3	30
35	Quantitative Assessment of Bâˆ’Bâˆ’B, Bâˆ’H_bâˆ’B, and Bâˆ’H_t Bonds: From BH₃ to B₁₂H₁₂^{2âˆ’}. ChemPhysChem, 2019, 20, 1967-1977.	2.1	30
36	Solving the Pericyclicâ€“Pseudopericyclic Puzzle in the Ring-Closure Reactions of 1,2,4,6-Heptatetraene Derivatives. Journal of Organic Chemistry, 2016, 81, 404-414.	3.2	29

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37	A Critical Evaluation of Vibrational Stark Effect (VSE) Probes with the Local Vibrational Mode Theory. Sensors, 2020, 20, 2358.	3.8	29
38	SSnet: A Deep Learning Approach for Protein-Ligand Interaction Prediction. International Journal of Molecular Sciences, 2021, 22, 1392.	4.1	29
39	Improved Predictorâ€“Corrector Integrators For Evaluating Reaction Path Curvature. Journal of Chemical Theory and Computation, 2013, 9, 1481-1488.	5.3	27
40	Local vibrational force constants â€“ From the assessment of empirical force constants to the description of bonding in large systems. Chemical Physics Letters, 2020, 748, 137337.	2.6	27
41	Predicting Potential SARS-COV-2 Drugsâ€”In Depth Drug Database Screening Using Deep Neural Network Framework SSnet, Classical Virtual Screening and Docking. International Journal of Molecular Sciences, 2021, 22, 1573.	4.1	27
42	Dieter Cremer's contribution to the field of theoretical chemistry. International Journal of Quantum Chemistry, 2019, 119, e25849.	2.0	26
43	Metalâ€“Halogen Bonding Seen through the Eyes of Vibrational Spectroscopy. Materials, 2020, 13, 55.	2.9	26
44	In Situ Assessment of Intrinsic Strength of X-Iâ‹¯OA-Type Halogen Bonds in Molecular Crystals with Periodic Local Vibrational Mode Theory. Molecules, 2020, 25, 1589.	3.8	26
45	Exceptionally Long Covalent CC Bondsâ€”A Local Vibrational Mode Study. Molecules, 2021, 26, 950.	3.8	26
46	Hydrogen Bonding in Natural and Unnatural Base Pairsâ€”A Local Vibrational Mode Study. Molecules, 2021, 26, 2268.	3.8	26
47	Chiral Discrimination by Vibrational Spectroscopy Utilizing Local Modes. Chirality, 2013, 25, 185-196.	2.6	25
48	Critical assessment of the FeC and CO bond strength in carboxymyoglobin: a QM/MM local vibrational mode study. Journal of Molecular Modeling, 2020, 26, 281.	1.8	24
49	The mechanism of the cycloaddition reaction of 1,3-dipole molecules with acetylene: an investigation with the unified reaction valley approach. Theoretical Chemistry Accounts, 2014, 133, 1.	1.4	23
50	Recovering Intrinsic Fragmental Vibrations Using the Generalized Subsystem Vibrational Analysis. Journal of Chemical Theory and Computation, 2018, 14, 2558-2569.	5.3	23
51	A stunning example for a spontaneous reaction with a complex mechanism: the vinylideneâ€“acetylene cycloaddition reaction. Molecular Physics, 2010, 108, 2667-2685.	1.7	22
52	Controlled Oxidation of an NHC-Stabilized Phosphinoaminosilylene with Dioxygen. Inorganic Chemistry, 2016, 55, 46-50.	4.0	22
53	New mechanistic insights into the Claisen rearrangement of chorismate â€“ a Unified Reaction Valley Approach study. Molecular Physics, 2019, 117, 1172-1192.	1.7	22
54	Local Vibrational Mode Analysis of Ï€â€“Hole Interactions between Aryl Donors and Small Molecule Acceptors. Crystals, 2020, 10, 556.	2.2	22

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55	Generative adversarial networks for transition state geometry prediction. Journal of Chemical Physics, 2021, 155, 024116.	3.0	21
56	Exploring the Mechanism of Catalysis with the Unified Reaction Valley Approach (URVA)â€"A Review. Catalysts, 2020, 10, 691.	3.5	20
57	Quantitative assessment of intramolecular hydrogen bonds in neutral histidine. Theoretical Chemistry Accounts, 2020, 139, 1.	1.4	20
58	Gold(I)-assisted catalysis â€“ a comprehensive view on the [3,3]-sigmatropic rearrangement of allyl acetate. Molecular Physics, 2018, 116, 611-630.	1.7	18
59	Uranium: The Nuclear Fuel Cycle and Beyond. International Journal of Molecular Sciences, 2022, 23, 4655.	4.1	18
60	Capturing Individual Hydrogen Bond Strengths in Ices via Periodic Local Vibrational Mode Theory: Beyond the Lattice Energy Picture. Journal of Chemical Theory and Computation, 2022, 18, 562-579.	5.3	17
61	Pushing 3câ€“4e Bonds to the Limit: A Coupled Cluster Study of Stepwise Fluorination of First-Row Atoms. Inorganic Chemistry, 2019, 58, 14777-14789.	4.0	16
62	A Sodaliteâ€Type Silver Orthophosphate Cluster in a Globular Silver Nanocluster. Angewandte Chemie, 2020, 132, 12759-12763.	2.0	16
63	Systematic description of molecular deformations with Cremerâ€“Pople puckering and deformation coordinates utilizing analytic derivatives: Applied to cycloheptane, cyclooctane, and cyclo[18]carbon. Journal of Chemical Physics, 2020, 152, 154107.	3.0	16
64	LModeA-nano: A PyMOL Plugin for Calculating Bond Strength in Solids, Surfaces, and Molecules via Local Vibrational Mode Analysis. Journal of Chemical Theory and Computation, 2022, 18, 1821-1837.	5.3	16
65	Characterizing Chemical Similarity with Vibrational Spectroscopy: New Insights into the Substituent Effects in Monosubstituted Benzenes. Journal of Physical Chemistry A, 2017, 121, 8086-8096.	2.5	15
66	Inverse folding with RNA-As-Graphs produces a large pool of candidate sequences with target topologies. Journal of Structural Biology, 2020, 209, 107438.	2.8	15
67	Systematic Detection and Characterization of Hydrogen Bonding in Proteins via Local Vibrational Modes. Journal of Physical Chemistry B, 2021, 125, 2551-2565.	2.6	15
68	PyVibMS: a PyMOL plugin for visualizing vibrations in molecules and solids. Journal of Molecular Modeling, 2020, 26, 290.	1.8	14
69	Local vibrational mode analysis of ionâ€“solvent and solventâ€“solvent interactions for hydrated Ca2+ clusters. Journal of Chemical Physics, 2020, 153, 224303.	3.0	14
70	Computational analysis of vibrational frequencies and rovibrational spectroscopic constants of hydrogen sulfide dimer using MP2 and CCSD(T). Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2020, 239, 118540.	3.9	14
71	Mechanosynthesis of a Coamorphous Formulation of Creatine with Citric Acid and Humidity-Mediated Transformation into a Cocrystal. Crystal Growth and Design, 2021, 21, 1297-1306.	3.0	14
72	Halogen Bonding Involving I2 and d8 Transition-Metal Pincer Complexes. Crystals, 2021, 11, 373.	2.2	14

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73	Metalâ€“ring interactions in actinide sandwich compounds: A combined normalized elimination of the small component and local vibrational mode study. Molecular Physics, 2020, 118, e1768314.	1.7	14
74	Observation of a bcc-like framework in polyhydrido copper nanoclusters. Nanoscale, 2021, 13, 19642-19649.	5.6	14
75	Modeling Hydrogen Release from Water with Borane and Alane Catalysts: A Unified Reaction Valley Approach. Journal of Physical Chemistry A, 2020, 124, 8978-8993.	2.5	12
76	Two Novel Palbociclib-Resorcinol and Palbociclib-Orcinol Cocrystals with Enhanced Solubility and Dissolution Rate. Pharmaceutics, 2022, 14, 23.	4.5	12
77	Correlating the vibrational spectra of structurally related molecules: A spectroscopic measure of similarity. Journal of Computational Chemistry, 2018, 39, 293-306.	3.3	11
78	Density functional theory study of selective aerobic oxidation of cyclohexane: the roles of acetic acid and cobalt ion. Journal of Molecular Modeling, 2019, 25, 71.	1.8	11
79	Theoretical Insights into [NHC]Au(I) Catalyzed Hydroalkoxylation of Allenes: A Unified Reaction Valley Approach Study. Journal of Organic Chemistry, 2021, 86, 5714-5726.	3.2	11
80	Comment on â€œExploring nature and predicting strength of hydrogen bonds: A correlation analysis between <scp>atomsâ€inâ€molecules</scp> descriptors, binding energies, and energy components of <scp>symmetryâ€adapted</scp> perturbation theoryâ€. Journal of Computational Chemistry, 2021, 42, 516-521.	3.3	9
81	Correlation between molecular acidity (pKa) and vibrational spectroscopy. Journal of Molecular Modeling, 2019, 25, 48.	1.8	8
82	Describing Polytopal Rearrangements of Fluxional Molecules with Curvilinear Coordinates Derived from Normal Vibrational Modes: A Conceptual Extension of Cremerâ€“Pople Puckering Coordinates. Journal of Chemical Theory and Computation, 2020, 16, 3162-3193.	5.3	8
83	Pivotal role of water molecules in the photodegradation of pymetrozine: New insights for developing green pesticides. Journal of Hazardous Materials, 2022, 423, 127197.	12.4	7
84	Structural study of 1- and 2-naphthol: new insights into the non-covalent Hâ€“H interaction in cis-1-naphthol. Physical Chemistry Chemical Physics, 2022, 24, 3722-3732.	2.8	7
85	Describing Polytopal Rearrangement Processes of Octacoordinate Structures. I. Renewed Insights into Fluxionality of the Rhenium Polyhydride Complex ReH₅(PPh₃)₂(Pyridine). Inorganic Chemistry, 2021, 60, 2492-2502.	4.0	6
86	A revised formulation of the generalized subsystem vibrational analysis (GSVA). Theoretical Chemistry Accounts, 2021, 140, 31.	1.4	6
87	Equilibrium Geometries, Adiabatic Excitation Energies and Intrinsic C=C/Câ€“H Bond Strengths of Ethylene in Lowest Singlet Excited States Described by TDDFT. Symmetry, 2020, 12, 1545.	2.2	5
88	Modified Density Functional Dispersion Correction for Inorganic Layered MFX Compounds (M = Ca, Sr,) Tj ETQq0 0 0 rgBT /Overlock 10	2.5	5
89	Assessing the Intrinsic Strengths of Ionâ€“Solvent and Solventâ€“Solvent Interactions for Hydrated Mg2+ Clusters. Inorganics, 2021, 9, 31.	2.7	5
90	Deep Learning-Based Ligand Design Using Shared Latent Implicit Fingerprints from Collaborative Filtering. Journal of Chemical Information and Modeling, 2021, 61, 2159-2174.	5.4	5

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91	Relating Bond Strength and Nature to the Thermodynamic Stability of Hypervalent Togniâ€Type Iodine Compounds. ChemPlusChem, 2021, 86, 1199-1210.	2.8	5
92	Preface: Dieter Cremer's scientific journey. Molecular Physics, 2019, 117, 1047-1058.	1.7	3
93	Characterizing the Metalâ€“Ligand Bond Strength via Vibrational Spectroscopy: The Metalâ€“Ligand Electronic Parameter (MLEP). Topics in Organometallic Chemistry, 2020, , 227-269.	0.7	3
94	Substituted hydrocarbon: a CCSD(T) and local vibrational mode investigation. Molecular Physics, 0, , e1970844.	1.7	3
95	BF3â€“Catalyzed Dielsâ€“Alder Reaction between Butadiene and Methyl Acrylate in Aqueous Solutionâ€”An URVA and Local Vibrational Mode Study. Catalysts, 2022, 12, 415.	3.5	3
96	Allosteric control of ACE2 peptidase domain dynamics. Organic and Biomolecular Chemistry, 2022, 20, 3605-3618.	2.8	3
97	On the formation of CN bonds in Titanâ€™s atmosphereâ€”a unified reaction valley approach study. Journal of Molecular Modeling, 2021, 27, 320.	1.8	2
98	A Closer Look at the Isomerization of 5-androstene-3,17-dione to 4-androstene-3,17-dione in Ketosteroid Isomerase. Journal of Computational Biophysics and Chemistry, 0, , 1-21.	1.7	2
99	Unusual Intramolecular Motion of ReH₉^{2â€“} in K₂ReH₉ Crystal: Circle Dance and Three-Arm Turnstile Mechanisms Revealed by Computational Studies. Inorganic Chemistry, 2022, 61, 1041-1050.	4.0	2
100	Crystal structure of 1-propanethiolâ€“Co2(dobdc) from laboratory X-ray powder diffraction data. Powder Diffraction, 2020, 35, 3-6.	0.2	1
101	Thermally Triggered Isomerization in a Naphthaleneâ€Based Acylhydrazone with Solidâ€State Optical Nonlinearity Response. European Journal of Inorganic Chemistry, 2020, 2020, 4313-4317.	2.0	1
102	Innentitelbild: A Sodaliteâ€Type Silver Orthophosphate Cluster in a Globular Silver Nanocluster (Angew. Chem. 31/2020). Angewandte Chemie, 2020, 132, 12646-12646.	2.0	0
103	Chemical Bonding in Homogenous Catalysis â€“ Seen Through the Eyes of Vibrational Spectroscopy. , 2024, , 622-648.		0