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 Bonding in Homogenous Catalysis â€“ Seen Through the Eyes of Vibrational Spectroscopy. , 2024, , 622-648.		0
2	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
3	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
4	Two Novel Palbociclib-Resorcinol and Palbociclib-Orcinol Cocrystals with Enhanced Solubility and Dissolution Rate. Pharmaceutics, 2022, 14, 23.	4.5	12
5	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
6	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
7	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
8	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
9	Allosteric control of ACE2 peptidase domain dynamics. Organic and Biomolecular Chemistry, 2022, 20, 3605-3618.	2.8	3
10	Uranium: The Nuclear Fuel Cycle and Beyond. International Journal of Molecular Sciences, 2022, 23, 4655.	4.1	18
11	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
12	SSnet: A Deep Learning Approach for Protein-Ligand Interaction Prediction. International Journal of Molecular Sciences, 2021, 22, 1392.	4.1	29
13	Exceptionally Long Covalent CC Bondsâ€”A Local Vibrational Mode Study. Molecules, 2021, 26, 950.	3.8	26
14	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
15	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
16	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
17	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
18	A revised formulation of the generalized subsystem vibrational analysis (GSVA). Theoretical Chemistry Accounts, 2021, 140, 31.	1.4	6

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19	Hydrogen Bonding in Natural and Unnatural Base Pairsâ€"A Local Vibrational Mode Study. Molecules, 2021, 26, 2268.	3.8	26
20	Assessing the Intrinsic Strengths of Ionâ€"Solvent and Solventâ€"Solvent Interactions for Hydrated Mg2+ Clusters. Inorganics, 2021, 9, 31.	2.7	5
21	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
22	Halogen Bonding Involving I2 and d8 Transition-Metal Pincer Complexes. Crystals, 2021, 11, 373.	2.2	14
23	Generative adversarial networks for transition state geometry prediction. Journal of Chemical Physics, 2021, 155, 024116.	3.0	21
24	Relating Bond Strength and Nature to the Thermodynamic Stability of Hypervalent Togniâ€Type Iodine Compounds. ChemPlusChem, 2021, 86, 1199-1210.	2.8	5
25	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
26	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
27	Observation of a bcc-like framework in polyhydrido copper nanoclusters. Nanoscale, 2021, 13, 19642-19649.	5.6	14
28	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
29	Metalâ€"Halogen Bonding Seen through the Eyes of Vibrational Spectroscopy. Materials, 2020, 13, 55.	2.9	26
30	PyVibMS: a PyMOL plugin for visualizing vibrations in molecules and solids. Journal of Molecular Modeling, 2020, 26, 290.	1.8	14
31	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
32	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
33	Machine learning of serum metabolic patterns encodes early-stage lung adenocarcinoma. Nature Communications, 2020, 11, 3556.	12.8	151
34	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
35	Local Vibrational Mode Analysis of Ï€â€"Hole Interactions between Aryl Donors and Small Molecule Acceptors. Crystals, 2020, 10, 556.	2.2	22
36	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

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37	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
38	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
39	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
40	A Sodaliteâ€Type Silver Orthophosphate Cluster in a Globular Silver Nanocluster. Angewandte Chemie, 2020, 132, 12759-12763.	2.0	16
41	Decoding chemical information from vibrational spectroscopy data: Local vibrational mode theory. Wiley Interdisciplinary Reviews: Computational Molecular Science, 2020, 10, e1480.	14.6	85
42	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
43	Chelation-Assisted Selective Etching Construction of Hierarchical Polyoxometalate-Based Metalâ€“Organic Framework. Chemistry of Materials, 2020, 32, 5550-5557.	6.7	43
44	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
45	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
46	Exploring the Mechanism of Catalysis with the Unified Reaction Valley Approach (URVA)â€”A Review. Catalysts, 2020, 10, 691.	3.5	20
47	Quantitative assessment of intramolecular hydrogen bonds in neutral histidine. Theoretical Chemistry Accounts, 2020, 139, 1.	1.4	20
48	Crystal structure of 1-propanethiolâ€“Co2(dobdc) from laboratory X-ray powder diffraction data. Powder Diffraction, 2020, 35, 3-6.	0.2	1
49	Modified Density Functional Dispersion Correction for Inorganic Layered MFX Compounds (M = Ca, Sr,) Tj ETQq1 1 0.784314 rgBT /O	2.5	5
50	A Critical Evaluation of Vibrational Stark Effect (VSE) Probes with the Local Vibrational Mode Theory. Sensors, 2020, 20, 2358.	3.8	29
51	A Sodaliteâ€Type Silver Orthophosphate Cluster in a Globular Silver Nanocluster. Angewandte Chemie - International Edition, 2020, 59, 12659-12663.	13.8	36
52	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
53	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
54	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

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55	Interplay of Ring Puckering and Hydrogen Bonding in Deoxyribonucleosides. Journal of Physical Chemistry A, 2019, 123, 7087-7103.	2.5	32
56	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
57	Preface: Dieter Cremer's scientific journey. Molecular Physics, 2019, 117, 1047-1058.	1.7	3
58	Correlation between molecular acidity (pKa) and vibrational spectroscopy. Journal of Molecular Modeling, 2019, 25, 48.	1.8	8
59	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
60	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
61	Quantitative Assessment of Bâ˜Bâ˜B, Bâ˜H_bâ˜B, and Bâ˜H_t Bonds: From BH₃ to B₁₂H₁₂^{2â˜}. ChemPhysChem, 2019, 20, 1967-1977.	2.1	30
62	Dieter Cremer's contribution to the field of theoretical chemistry. International Journal of Quantum Chemistry, 2019, 119, e25849.	2.0	26
63	A Continuum from Halogen Bonds to Covalent Bonds: Where Do Î»3 Iodanes Fit?. Inorganics, 2019, 7, 47.	2.7	39
64	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
65	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
66	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
67	Recovering Intrinsic Fragmental Vibrations Using the Generalized Subsystem Vibrational Analysis. Journal of Chemical Theory and Computation, 2018, 14, 2558-2569.	5.3	23
68	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
69	Correlating the vibrational spectra of structurally related molecules: A spectroscopic measure of similarity. Journal of Computational Chemistry, 2018, 39, 293-306.	3.3	11
70	Quantitative Assessment of Tetrel Bonding Utilizing Vibrational Spectroscopy. Molecules, 2018, 23, 2763.	3.8	84
71	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
72	Quantitative Assessment of Halogen Bonding Utilizing Vibrational Spectroscopy. Inorganic Chemistry, 2017, 56, 488-502.	4.0	91

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73	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
74	Strengthening of hydrogen bonding with the push-pull effect. Chemical Physics Letters, 2017, 685, 251-258.	2.6	58
75	The Many Facets of Chalcogen Bonding: Described by Vibrational Spectroscopy. Journal of Physical Chemistry A, 2017, 121, 6845-6862.	2.5	95
76	Systematic Coupled Cluster Study of Noncovalent Interactions Involving Halogens, Chalcogens, and Pnicogens. Journal of Physical Chemistry A, 2017, 121, 9544-9556.	2.5	72
77	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
78	Quantitative Assessment of Aromaticity and Antiaromaticity Utilizing Vibrational Spectroscopy. Journal of Organic Chemistry, 2016, 81, 9669-9686.	3.2	56
79	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
80	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
81	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
82	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
83	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
84	Direct Measure of Metalâ€“Ligand Bonding Replacing the Tolman Electronic Parameter. Inorganic Chemistry, 2016, 55, 2332-2344.	4.0	85
85	Controlled Oxidation of an NHC-Stabilized Phosphinoaminosilylene with Dioxygen. Inorganic Chemistry, 2016, 55, 46-50.	4.0	22
86	Hidden Bond Anomalies: The Peculiar Case of the Fluorinated Amine Chalcogenides. Journal of Physical Chemistry A, 2015, 119, 9541-9556.	2.5	54
87	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
88	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
89	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
90	Enediynes, enyneâ€allenes, their reactions, and beyond. Wiley Interdisciplinary Reviews: Computational Molecular Science, 2014, 4, 285-324.	14.6	32

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91	Are carbonâ€"halogen double and triple bonds possible?. International Journal of Quantum Chemistry, 2014, 114, 1060-1072.	2.0	41
92	Identification of the Strongest Bonds in Chemistry. Journal of Physical Chemistry A, 2013, 117, 8981-8995.	2.5	140
93	Improved Predictorâ€"Corrector Integrators For Evaluating Reaction Path Curvature. Journal of Chemical Theory and Computation, 2013, 9, 1481-1488.	5.3	27
94	Chiral Discrimination by Vibrational Spectroscopy Utilizing Local Modes. Chirality, 2013, 25, 185-196.	2.6	25
95	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
96	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
97	A comprehensive analysis of hydrogen bond interactions based on local vibrational modes. International Journal of Quantum Chemistry, 2012, 112, 3174-3187.	2.0	121
98	Reaction path Hamiltonian and the unified reaction valley approach. Wiley Interdisciplinary Reviews: Computational Molecular Science, 2011, 1, 531-556.	14.6	47
99	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
100	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
101	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
102	Substituted hydrocarbon: a CCSD(T) and local vibrational mode investigation. Molecular Physics, 0, , e1970844.	1.7	3
103	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