

Comprehensive Thermochemical Benchmark Set of Reactions

Journal of Chemical Theory and Computation

14, 2596-2608

DOI: [10.1021/acs.jctc.7b01183](https://doi.org/10.1021/acs.jctc.7b01183)

Citation Report

#	ARTICLE	IF	CITATIONS
5	Accuracy of theoretical catalysis from a model of iron-catalyzed ammonia synthesis. <i>Communications Chemistry</i> , 2018, 1, .	2.0	11
6	Insight into mechanism of iron-oxides reduction in atmospheres of CH ₄ and CO. <i>Chemical Physics Letters</i> , 2018, 706, 708-714.	1.2	8
7	Formulation of Small Test Sets Using Large Test Sets for Efficient Assessment of Quantum Chemistry Methods. <i>Journal of Chemical Theory and Computation</i> , 2018, 14, 4254-4262.	2.3	25
8	M11plus: A Range-Separated Hybrid Meta Functional with Both Local and Rung-3.5 Correlation Terms and High Across-the-Board Accuracy for Chemical Applications. <i>Journal of Chemical Theory and Computation</i> , 2019, 15, 4804-4815.	2.3	24
9	Intermetallic species in the Negishi coupling and their involvement in inhibition pathways. <i>Catalysis Science and Technology</i> , 2019, 9, 4561-4572.	2.1	8
10	Mechanism and Control of the Palladium-Catalyzed Alkoxy-carbonylation of Oleochemicals from Sustainable Sources. <i>ChemCatChem</i> , 2019, 11, 4894-4906.	1.8	13
11	Ï%B2PLYP and Ï%B2GPPLYP: The First Two Double-Hybrid Density Functionals with Long-Range Correction Optimized for Excitation Energies. <i>Journal of Chemical Theory and Computation</i> , 2019, 15, 4735-4744.	2.3	107
12	A Benchmark of Density Functional Approximations For Thermochemistry and Kinetics of Hydride Reductions of Cyclohexanones. <i>ChemistryOpen</i> , 2019, 8, 788-806.	0.9	7
13	Thermodynamics of H ⁺ /H [•] /H [•] /H [•] /e [•] Transfer from [CpV(CO) ₃ H] [•] : Comparisons to the Isoelectronic CpCr(CO) ₃ H. <i>Organometallics</i> , 2019, 38, 4319-4328.	1.1	10
14	Interaction between water and carbon nanostructures: How good are current density functional approximations?. <i>Journal of Chemical Physics</i> , 2019, 151, 164702.	1.2	47
15	Copper hydride-mediated electrophilic amidation of vinylarenes with dioxazolones – a computational mechanistic study. <i>Dalton Transactions</i> , 2019, 48, 14337-14346.	1.6	4
16	A noncovalent interaction insight onto the concerted metallation deprotonation mechanism. <i>Physical Chemistry Chemical Physics</i> , 2019, 21, 20486-20498.	1.3	17
17	Molecularly Defined Manganese Catalyst for Low-Temperature Hydrogenation of Carbon Monoxide to Methanol. <i>Journal of the American Chemical Society</i> , 2019, 141, 16923-16929.	6.6	62
18	Extremely large differences in DFT energies for nitrogenase models. <i>Physical Chemistry Chemical Physics</i> , 2019, 21, 2480-2488.	1.3	56
19	Face-Sharing Homo- and Hetero-Bitetrahedral Superatomic Molecules M ₁ M ₂ @Li ₂₀ (M ₁ /M ₂ = Ti and W). <i>Journal of Physical Chemistry A</i> , 2019, 123, 5517-5524.	1.1	6
20	Structure Optimisation of Large Transition-Metal Complexes with Extended Tight-Binding Methods. <i>Angewandte Chemie - International Edition</i> , 2019, 58, 11078-11087.	7.2	72
21	Minimally Empirical Double-Hybrid Functionals Trained against the GMTKN55 Database: revDSD-PBEP86-D4, revDOD-PBE-D4, and DOD-SCAN-D4. <i>Journal of Physical Chemistry A</i> , 2019, 123, 5129-5143.	1.1	262
22	Assessment of DFT Methods for Transition Metals with the TMC151 Compilation of Data Sets and Comparison with Accuracies for Main-Group Chemistry. <i>Journal of Chemical Theory and Computation</i> , 2019, 15, 3610-3622.	2.3	85

#	ARTICLE	IF	CITATIONS
23	Structure Optimisation of Large Transition-Metal Complexes with Extended Tight-Binding Methods. <i>Angewandte Chemie</i> , 2019, 131, 11195-11204.	1.6	21
24	On the structures of dinuclear symmetric lanthanide complexes and the selectivity towards heterodinuclear complexes based on molecular modeling. <i>Inorganica Chimica Acta</i> , 2019, 494, 65-73.	1.2	13
25	Ethylene glycol as an efficient and reversible liquid-organic hydrogen carrier. <i>Nature Catalysis</i> , 2019, 2, 415-422.	16.1	102
26	A generally applicable atomic-charge dependent London dispersion correction. <i>Journal of Chemical Physics</i> , 2019, 150, 154122.	1.2	697
27	Evaluating Transition Metal Barrier Heights with the Latest Density Functional Theory Exchange-Correlation Functionals: The MOBH35 Benchmark Database. <i>Journal of Physical Chemistry A</i> , 2019, 123, 3761-3781.	1.1	104
28	GFN2-xTB-An Accurate and Broadly Parametrized Self-Consistent Tight-Binding Quantum Chemical Method with Multipole Electrostatics and Density-Dependent Dispersion Contributions. <i>Journal of Chemical Theory and Computation</i> , 2019, 15, 1652-1671.	2.3	1,704
29	Emerging DFT Methods and Their Importance for Challenging Molecular Systems with Orbital Degeneracy. <i>Computation</i> , 2019, 7, 62.	1.0	5
30	Coupled cluster benchmark of new density functionals and of domain pair natural orbital methods: Mechanisms of hydroarylation and oxidative coupling catalyzed by Ru(II) chloride carbonyls. <i>AIP Conference Proceedings</i> , 2019, , .	0.3	10
31	ACCCDB: A collection of chemistry databases for broad computational purposes. <i>Journal of Computational Chemistry</i> , 2019, 40, 839-848.	1.5	42
32	Understanding and Quantifying London Dispersion Effects in Organometallic Complexes. <i>Accounts of Chemical Research</i> , 2019, 52, 258-266.	7.6	117
33	Assessment of Initial Guesses for Self-Consistent Field Calculations. Superposition of Atomic Potentials: Simple yet Efficient. <i>Journal of Chemical Theory and Computation</i> , 2019, 15, 1593-1604.	2.3	37
34	Structures and binding energies for complexations of different spin states of Ni ⁺ and Ni ²⁺ to aromatic molecules. <i>Molecular Physics</i> , 2019, 117, 1392-1403.	0.8	4
35	Odd-even effect of the number of free valence electrons on the electronic structure properties of gold-thiolate clusters. <i>Molecular Physics</i> , 2019, 117, 1442-1450.	0.8	5
36	Superatomic properties of transition-metal-doped tetrahedral lithium clusters: TM@Li ₄ . <i>Molecular Physics</i> , 2020, 118, e1592256.	0.8	9
37	The finding of transition-metal-doped binary superatoms: TM@Li ₁₅ . <i>Journal of Physics B: Atomic, Molecular and Optical Physics</i> , 2020, 53, 015101.	0.6	1
38	Formation of Mn hydrides from bis(trimethylsilylmethyl) Mn(II): A DFT study. <i>Polyhedron</i> , 2020, 178, 114355.	1.0	0
39	Isomerism and dynamic behavior of bridging phosphalkynes bound to a dicopper complex. <i>Chemical Science</i> , 2020, 11, 1607-1616.	3.7	11
40	Electronic structure calculations permit identification of the driving forces behind frequency shifts in transition metal monocarbonyls. <i>Physical Chemistry Chemical Physics</i> , 2020, 22, 781-798.	1.3	21

#	ARTICLE	IF	CITATIONS
41	A coumarin derivative-Cu ²⁺ complex-based fluorescent chemosensor for detection of biothiols. RSC Advances, 2020, 10, 36265-36274.	1.7	8
42	Density Functional Theories and Coordination Chemistry. , 2020, , .		2
43	Reactivity of arsenoplatin complex versus water and thiocyanate: a DFT benchmark study. Theoretical Chemistry Accounts, 2020, 139, 1.	0.5	19
44	Computational chemistry considerations in catalysis: Regioselectivity and metal-ligand dissociation. Catalysis Today, 2020, 358, 422-429.	2.2	5
45	Benchmark study of density functionals for the insertions of olefin and polar monomers catalyzed by σ -diimine palladium complexes. Computational and Theoretical Chemistry, 2020, 1187, 112942.	1.1	3
46	DFT counterparts of leading generalized gradient approximation and hybrid density functionals for energetics and geometries. Journal of Computational Chemistry, 2020, 41, 2562-2572.	1.5	61
47	Reactivity-Controlling Factors in Carboxylate-Assisted C-H Activation under 4d and 3d Transition Metal Catalysis. ACS Catalysis, 2020, 10, 10551-10558.	5.5	69
48	On the Structure of Intermediates in Enyne Gold(I)-Catalyzed Cyclizations: Formation of <i>trans</i> -Fused Bicyclo[5.1.0]octanes as a Case Study. Chemistry - A European Journal, 2020, 26, 15738-15745.	1.7	12
49	Probabilistic performance estimators for computational chemistry methods: Systematic improvement probability and ranking probability matrix. II. Applications. Journal of Chemical Physics, 2020, 152, 164109.	1.2	7
50	Tuning the Reactivity and Bonding Properties of Metal Square-Planar Complexes by the Substitution(s) on the Trans-Coordinated Pyridine Ring. ACS Omega, 2020, 5, 11768-11783.	1.6	9
51	On the Nature of C(sp ³)-C(sp ²) Bond Formation in Nickel-Catalyzed Tertiary Radical Cross-Couplings: A Case Study of Ni/Photoredox Catalytic Cross-Coupling of Alkyl Radicals and Aryl Halides. Journal of the American Chemical Society, 2020, 142, 7225-7234.	6.6	151
52	Engaging α -Fluorocarboxylic Acids Directly in Decarboxylative C-C Bond Formation. ACS Catalysis, 2020, 10, 4451-4459.	5.5	27
53	M11plus, a Range-Separated Hybrid Meta Functional Incorporating Nonlocal Rung-3.5 Correlation, Exhibits Broad Accuracy on Diverse Databases. Journal of Physical Chemistry Letters, 2020, 11, 3045-3050.	2.1	10
54	Semiautomated Transition State Localization for Organometallic Complexes with Semiempirical Quantum Chemical Methods. Journal of Chemical Theory and Computation, 2020, 16, 2002-2012.	2.3	60
55	Metal-Ligand Cooperativity in Titanium-Catalyzed Anti-Markovnikov Hydroamination. ACS Catalysis, 2020, 10, 7100-7111.	5.5	12
56	Status and Challenges of Density Functional Theory. Trends in Chemistry, 2020, 2, 302-318.	4.4	216
57	Efficient alkene hydrosilation with bis(8-quinolyl)phosphine (NPN) nickel catalysts. The dominant role of silyl-over hydrido-nickel catalytic intermediates. Chemical Science, 2020, 11, 5043-5051.	3.7	7
58	Double hybrid DFT calculations with Slater type orbitals. Journal of Computational Chemistry, 2020, 41, 1660-1684.	1.5	16

#	ARTICLE	IF	CITATIONS
59	Predicting Ligand-Dissociation Energies of 3d Coordination Complexes with Auxiliary-Field Quantum Monte Carlo. <i>Journal of Chemical Theory and Computation</i> , 2020, 16, 3041-3054.	2.3	21
60	On the top rung of Jacob's ladder of density functional theory: Toward resolving the dilemma of $\langle \text{SIE} \rangle$ and $\langle \text{NCE} \rangle$. <i>Wiley Interdisciplinary Reviews: Computational Molecular Science</i> , 2021, 11, .	6.2	25
61	Extended $\langle \text{tight-binding} \rangle$ quantum chemistry methods. <i>Wiley Interdisciplinary Reviews: Computational Molecular Science</i> , 2021, 11, e1493.	6.2	596
62	Theoretical study on conformational energies of transition metal complexes. <i>Physical Chemistry Chemical Physics</i> , 2021, 23, 287-299.	1.3	52
63	The magnetic binary lithium clusters W_2Li_n ($n = 15$ – 19): A theoretical prediction of $\langle \text{superatomic molecules} \rangle$. <i>International Journal of Quantum Chemistry</i> , 2021, 121, e26434.	1.0	2
64	Theoretical modeling of the singlet–triplet spin transition in different Ni($\langle \text{ii} \rangle$)-diketo-pyrphyrin-based metal–ligand octahedral complexes. <i>Physical Chemistry Chemical Physics</i> , 2021, 23, 4784-4795.	1.3	1
65	Calculation of absolute molecular entropies and heat capacities made simple. <i>Chemical Science</i> , 2021, 12, 6551-6568.	3.7	83
66	Accurate Reduced-Cost CCSD(T) Energies: Parallel Implementation, Benchmarks, and Large-Scale Applications. <i>Journal of Chemical Theory and Computation</i> , 2021, 17, 860-878.	2.3	32
67	High denticity oxinate-linear-backbone chelating ligand for diagnostic radiometal ions $[\text{111In}]\text{In}^{3+}$ and $[\text{89Zr}]\text{Zr}^{4+}$. <i>Dalton Transactions</i> , 2021, 50, 3874-3886.	1.6	7
68	The DFT study on pentannulation reaction of tungsten Fischer carbene complexes. <i>Computational and Theoretical Chemistry</i> , 2021, 1196, 113121.	1.1	0
69	Unexpected Substituent Effects in Aryl-Aryl Negishi Cross-Coupling Reactions Rationalized by Density Functional Theory and Natural Charges. <i>Organometallics</i> , 2021, 40, 591-599.	1.1	3
70	r2SCAN-3c: A $\langle \text{Swiss army knife} \rangle$ -composite electronic-structure method. <i>Journal of Chemical Physics</i> , 2021, 154, 064103.	1.2	290
71	r2SCAN-D4: Dispersion corrected meta-generalized gradient approximation for general chemical applications. <i>Journal of Chemical Physics</i> , 2021, 154, 061101.	1.2	70
72	Too big, too small, or just right? A benchmark assessment of density functional theory for predicting the spatial extent of the electron density of small chemical systems. <i>Journal of Chemical Physics</i> , 2021, 154, 074109.	1.2	15
73	Phosphonate Chelators for Medicinal Metal Ions. <i>Inorganic Chemistry</i> , 2021, 60, 5343-5361.	1.9	15
74	Solvent effects in hydroformylation of long-chain olefins. <i>Molecular Catalysis</i> , 2021, 503, 111429.	1.0	4
75	Exploring Avenues beyond Revised DSD Functionals: II. Random-Phase Approximation and Scaled MP3 Corrections. <i>Journal of Physical Chemistry A</i> , 2021, 125, 4628-4638.	1.1	12
76	Revealing the nature of electron correlation in transition metal complexes with symmetry breaking and chemical intuition. <i>Journal of Chemical Physics</i> , 2021, 154, 194109.	1.2	36

#	ARTICLE	IF	CITATIONS
77	OO-REMP: Approaching Chemical Accuracy with Second-Order Perturbation Theory. <i>Journal of Chemical Theory and Computation</i> , 2021, 17, 3259-3266.	2.3	3
78	Efficient Computation of Geometries for Gold Complexes. <i>ChemPhysChem</i> , 2021, 22, 1262-1268.	1.0	4
80	Multiwavelets applied to metal–ligand interactions: Energies free from basis set errors. <i>Journal of Chemical Physics</i> , 2021, 154, 214302.	1.2	5
81	Robust and Efficient Implicit Solvation Model for Fast Semiempirical Methods. <i>Journal of Chemical Theory and Computation</i> , 2021, 17, 4250-4261.	2.3	186
82	A Massively Parallel Implementation of the CCSD(T) Method Using the Resolution-of-the-Identity Approximation and a Hybrid Distributed/Shared Memory Parallelization Model. <i>Journal of Chemical Theory and Computation</i> , 2021, 17, 4799-4822.	2.3	23
83	Multilevel approach to the initial guess for self-consistent field calculations. <i>International Journal of Quantum Chemistry</i> , 2022, 122, e26782.	1.0	3
84	Magnetic superatoms in cage doped 13-atom trimetallic Mg _n Li ₁₂ Sc _n (n = 1–3). <i>Physica B: Atomic, Molecular and Optical Physics</i> , 2021, 54, 145005.	0.6	0
85	Computational Discovery of Transition-metal Complexes: From High-throughput Screening to Machine Learning. <i>Chemical Reviews</i> , 2021, 121, 9927-10000.	23.0	110
86	Software for the frontiers of quantum chemistry: An overview of developments in the Q-Chem 5 package. <i>Journal of Chemical Physics</i> , 2021, 155, 084801.	1.2	518
87	Quantum chemical calculations of lithium-ion battery electrolyte and interphase species. <i>Scientific Data</i> , 2021, 8, 203.	2.4	19
88	Comparison of the accuracy of DFT methods for reactions with relevance to nitrogenase. <i>Electronic Structure</i> , 2021, 3, 034005.	1.0	9
89	Data-Driven Prediction of Formation Mechanisms of Lithium Ethylene Monocarbonate with an Automated Reaction Network. <i>Journal of the American Chemical Society</i> , 2021, 143, 13245-13258.	6.6	29
90	An improved chain of spheres for exchange algorithm. <i>Journal of Chemical Physics</i> , 2021, 155, 104109.	1.2	64
91	Assessing Density Functional Theory for Chemically Relevant Open-Shell Transition Metal Reactions. <i>Journal of Chemical Theory and Computation</i> , 2021, 17, 6134-6151.	2.3	75
92	Surprisingly Good Performance of XYG3 Family Functionals Using a Scaled KS-MP3 Correlation. <i>Journal of Physical Chemistry Letters</i> , 2021, 12, 9368-9376.	2.1	7
93	Benchmark test of a dispersion corrected revised Tao–Mo semilocal functional for thermochemistry, kinetics, and noncovalent interactions of molecules and solids. <i>Journal of Chemical Physics</i> , 2021, 155, 114102.	1.2	4
94	Coupled Cluster Benchmark of New DFT and Local Correlation Methods: Mechanisms of Hydroarylation and Oxidative Coupling Catalyzed by Ru(II, III) Chloride Carbonyls. <i>Journal of Physical Chemistry A</i> , 2021, 125, 8987-8999.	1.1	22
95	Reactivity of antitumor coinage metal-based N-heterocyclic carbene complexes with cysteine and selenocysteine protein sites. <i>Journal of Inorganic Biochemistry</i> , 2021, 223, 111533.	1.5	22

#	ARTICLE	IF	CITATIONS
96	Non-palindromic (C ^C D) gold(ⁱⁱⁱ) pincer complexes are not accessible by intramolecular oxidative addition of biphenylenes – an experimental and quantum chemical study. Dalton Transactions, 2021, 50, 9754-9767.	1.6	4
97	Influence of linkers on the Kuratowski-type secondary building unit in nickel single-site MOFs for ethylene oligomerization catalysis: a computational study. Catalysis Science and Technology, 2021, 11, 2422-2432.	2.1	9
98	Molecular dynamics simulation of the Pb(II) coordination in biological media via cationic dummy atom models. Theoretical Chemistry Accounts, 2021, 140, 1.	0.5	19
99	Novel hybrids based on graphene quantum dots covalently linked to glycol corroles for multiphoton bioimaging. Carbon, 2020, 166, 164-174.	5.4	39
100	Dynamics of nuclear recoil: QM-BOMD simulations of model systems following I ² -decay. Physical Chemistry Chemical Physics, 2021, 23, 25689-25698.	1.3	3
101	Chemical accuracy with <i>if</i> -functionals for the Kohn–Sham correlation energy optimized for different input orbitals and eigenvalues. Journal of Chemical Physics, 2021, 155, 134111.	1.2	14
102	Do Double-Hybrid Exchange–Correlation Functionals Provide Accurate Chemical Shifts? A Benchmark Assessment for Proton NMR. Journal of Chemical Theory and Computation, 2021, 17, 6876-6885.	2.3	34
103	A simplistic computational procedure for tunneling splittings caused by proton transfer. Structural Chemistry, 2022, 33, 351-362.	1.0	7
105	Reaction of dirhodium and diruthenium paddlewheel tetraacetate complexes with nucleophilic protein sites: A computational study. Inorganica Chimica Acta, 2022, 530, 120684.	1.2	16
106	Computational strategies to model the interaction and the reactivity of biologically-relevant transition metal complexes. Inorganica Chimica Acta, 2022, 530, 120686.	1.2	20
108	Transforming CO ₂ into Methanol with N-Heterocyclic Carbene-Stabilized Coinage Metal Hydrides Immobilized in a Metal–Organic Framework UiO-68. ACS Applied Materials & Interfaces, 2021, 13, 58723-58736.	4.0	18
109	The many roles of solvent in homogeneous catalysis - The reductive amination showcase. Journal of Catalysis, 2022, 405, 24-34.	3.1	8
110	The MOBH35 Metal–Organic Barrier Heights Reconsidered: Performance of Local-Orbital Coupled Cluster Approaches in Different Static Correlation Regimes. Journal of Chemical Theory and Computation, 2022, 18, 883-898.	2.3	27
111	Mechanism and Stereochemistry of Rhodium-Catalyzed [5 + 2 + 1] Cycloaddition of Ene–Vinylcyclopropanes and Carbon Monoxide Revealed by Visual Kinetic Analysis and Quantum Chemical Calculations. Journal of the American Chemical Society, 2022, 144, 2624-2636.	6.6	21
112	A general justification for hybrid functionals in DFT by means of linear response theory*. Journal of Physics Condensed Matter, 2022, 34, 194004.	0.7	0
113	Regularized Second-Order Møller–Plesset Theory: A More Accurate Alternative to Conventional MP2 for Noncovalent Interactions and Transition Metal Thermochemistry for the Same Computational Cost. Journal of Physical Chemistry Letters, 2021, 12, 12084-12097.	2.1	32
114	Density Functional Theory for Transition Metal Catalysis. , 2024, , 562-585.		0
115	New Mechanistic Insights into the Ru–Catalyzed Asymmetric Hydrogenation of I ² –Ketoesters. European Journal of Organic Chemistry, 0, , .	1.2	1

#	ARTICLE	IF	CITATIONS
116	Dispersion corrected r2SCAN based global hybrid functionals: r2SCANh, r2SCAN0, and r2SCAN50. <i>Journal of Chemical Physics</i> , 2022, 156, 134105.	1.2	32
117	Calculation of Metallocene Ionization Potentials via Auxiliary Field Quantum Monte Carlo: Toward Benchmark Quantum Chemistry for Transition Metals. <i>Journal of Chemical Theory and Computation</i> , 2022, 18, 2845-2862.	2.3	18
118	In Vitro Anti-SARS-CoV-2 Activity of Selected Metal Compounds and Potential Molecular Basis for Their Actions Based on Computational Study. <i>Biomolecules</i> , 2021, 11, 1858.	1.8	11
119	Reactivity of N-Heterocyclic Carbene Half-Sandwich Ru-, Os-, Rh-, and Ir-Based Complexes with Cysteine and Selenocysteine: A Computational Study. <i>Inorganic Chemistry</i> , 2022, 61, 746-754.	1.9	13
120	Molecule-Specific Uncertainty Quantification in Quantum Chemical Studies. <i>Israel Journal of Chemistry</i> , 2022, 62, .	1.0	16
121	Oxidation State Localized Orbitals: A Method for Assigning Oxidation States Using Optimally Fragment-Localized Orbitals and a Fragment Orbital Localization Index. <i>Journal of Chemical Theory and Computation</i> , 2022, 18, 309-322.	2.3	16
122	BH9, a New Comprehensive Benchmark Data Set for Barrier Heights and Reaction Energies: Assessment of Density Functional Approximations and Basis Set Incompleteness Potentials. <i>Journal of Chemical Theory and Computation</i> , 2022, 18, 151-166.	2.3	27
123	Do Double-Hybrid Functionals Benefit from Regularization in the PT2 Term? Observations from an Extensive Benchmark. <i>Journal of Physical Chemistry Letters</i> , 2022, 13, 3499-3506.	2.1	14
124	Comparative Study of Vibrational Raman Optical Activity with Different Time-Dependent Density Functional Approximations: The VROA36 Database. <i>Journal of Physical Chemistry A</i> , 2022, 126, 2909-2927.	1.1	4
125	A Localized-Orbital Energy Evaluation for Auxiliary-Field Quantum Monte Carlo. <i>Journal of Chemical Theory and Computation</i> , 2022, 18, 3447-3459.	2.3	7
126	Calculation of electric field gradients for CdI2 in the gas phase using BOMD simulations. <i>Chemical Physics Letters</i> , 2022, 801, 139704.	1.2	1
127	Theoretical Study on the Mechanism of the Carbonylation Cyclization of 1,5-Diynes with Hydrosilanes. <i>SSRN Electronic Journal</i> , 0, , .	0.4	0
128	Optimization of the r ² SCAN-3c Composite Electronic-Structure Method for Use with Slater-Type Orbital Basis Sets. <i>Journal of Physical Chemistry A</i> , 2022, 126, 3826-3838.	1.1	8
129	Better force fields start with better data: A data set of cation dipeptide interactions. <i>Scientific Data</i> , 2022, 9, .	2.4	5
130	Site-Selective C [~] H Arylation of Diverse Arenes Ortho to Small Alkyl Groups. <i>Angewandte Chemie - International Edition</i> , 2022, 61, .	7.2	6
131	Mechanistic Studies and Data Science-Guided Exploration of Bromotetrazine Cross-Coupling. <i>ACS Catalysis</i> , 2022, 12, 9226-9237.	5.5	5
132	Site-Selective C [~] H Arylation of Diverse Arenes Ortho to Small Alkyl Groups. <i>Angewandte Chemie</i> , 0, , .	1.6	0
133	A Look at Real-World Transition-Metal Thermochemistry and Kinetics with Local Hybrid Functionals. <i>Israel Journal of Chemistry</i> , 2023, 63, .	1.0	8

#	ARTICLE	IF	CITATIONS
134	Coordination-Induced Weakening of a C(sp ³)-H Bond: Homolytic and Heterolytic Bond Strength of a CH ₃ -Ni Agostic Interaction. <i>Journal of the American Chemical Society</i> , 2022, 144, 12632-12637.	6.6	4
135	Exploring the Reaction Mechanism of C-H Oxidation by Copper-Salen Complexes. <i>Journal of Physical Chemistry A</i> , 0, .	1.1	0
136	An assessment of orbital energy corrections for the direct random phase approximation and explicit <i>r</i> -functionals. <i>Molecular Physics</i> , 0, .	0.8	5
137	Benefits of Range-Separated Hybrid and Double-Hybrid Functionals for a Large and Diverse Data Set of Reaction Energies and Barrier Heights. <i>Journal of Physical Chemistry A</i> , 2022, 126, 5492-5505.	1.1	11
138	Highly efficient CO ₂ conversion on a robust metal-organic framework Cu(I)-MFU-4l: Prediction and mechanistic understanding from DFT calculations. <i>Journal of CO₂ Utilization</i> , 2022, 63, 102148.	3.3	1
139	Theoretical study on the mechanism of the carbonylation cyclization of 1,5-diyne with hydrosilanes. <i>Journal of Organometallic Chemistry</i> , 2022, 979, 122481.	0.8	0
140	DFT exchange: sharing perspectives on the workhorse of quantum chemistry and materials science. <i>Physical Chemistry Chemical Physics</i> , 2022, 24, 28700-28781.	1.3	91
141	Structural Reshaping of the Zinc-Finger Domain of the SARS-CoV-2 nsp13 Protein Using Bismuth(III) Ions: A Multilevel Computational Study. <i>Inorganic Chemistry</i> , 2022, 61, 15664-15677.	1.9	9
142	Scaled <i>r</i> -functionals for the Kohn-Sham correlation energy with scaling functions from the homogeneous electron gas. <i>Journal of Chemical Physics</i> , 2022, 157, .	1.2	8
143	Best-Practice DFT Protocols for Basic Molecular Computational Chemistry**. <i>Angewandte Chemie</i> , 2022, 134, .	1.6	36
144	Best-Practice DFT Protocols for Basic Molecular Computational Chemistry**. <i>Angewandte Chemie - International Edition</i> , 2022, 61, .	7.2	168
145	Metal Confined in 2D Membranes for Molecular Recognition and Sieving towards Ethylene/Ethane Separation. <i>Advanced Materials</i> , 2022, 34, .	11.1	21
146	Nitrogen atom coordination tuned transition metal catalysts for NO oxidation and reduction. <i>Chemosphere</i> , 2022, , 136735.	4.2	1
147	Theoretical investigation on interactions between N-methylpyrrolidone-FeCl ₃ and components in model oil: The role of S-Fe coordination in thiophene removal. <i>Journal of Molecular Liquids</i> , 2022, 368, 120719.	2.3	4
148	Rational Design of Metal-Alkoxide-Functionalized Metal-Organic Frameworks for Synergistic Dual Activation of CH ₄ and CO ₂ toward Acetic Acid Synthesis. <i>ACS Applied Materials & Interfaces</i> , 2022, 14, 52979-52992.	4.0	2
149	Influence of the complete basis set approximation, tight weighted-core, and diffuse functions on the <i>DLPNO-CCSD(T)</i> atomization energies of neutral H,C,O-compounds. <i>Journal of Computational Chemistry</i> , 2023, 44, 687-696.	1.5	2
150	A comprehensive benchmark investigation of quantum chemical methods for carbocations. <i>Physical Chemistry Chemical Physics</i> , 2023, 25, 1903-1922.	1.3	3
151	Faster Exact Exchange for Solids via occ-RI-K: Application to Combinatorially Optimized Range-Separated Hybrid Functionals for Simple Solids with Pseudopotentials Near the Basis Set Limit. <i>Journal of Chemical Theory and Computation</i> , 2022, 18, 7336-7349.	2.3	10

#	ARTICLE	IF	CITATIONS
152	<i>h</i> B97X-3c: A composite range-separated hybrid DFT method with a molecule-optimized polarized valence double- <i>h</i> basis set. <i>Journal of Chemical Physics</i> , 2023, 158, .	1.2	18
153	Inorganic Drugs as a Tool for Protein Structure Solving and Studies on Conformational Changes. <i>Chemistry - A European Journal</i> , 2023, 29, .	1.7	0
154	Full Implementation, Optimization, and Evaluation of a Range-Separated Local Hybrid Functional with Wide Accuracy for Ground and Excited States. <i>Journal of Chemical Theory and Computation</i> , 2023, 19, 488-502.	2.3	14
155	On the accuracy of orbital based multi-level approaches for closed-shell transition metal chemistry. <i>Physical Chemistry Chemical Physics</i> , 2023, 25, 4635-4648.	1.3	3
156	Accelerating computations of organometallic reaction energies through hybrid basis sets. <i>Inorganic Chemistry Frontiers</i> , 2023, 10, 2262-2267.	3.0	0
157	Computational Modeling of 4d and 5d Transition Metal Catalysts. , 2024, , 601-621.		0
158	Finite-Temperature Mechanical Properties of Organic Molecular Crystals from Classical Molecular Simulation. <i>Crystal Growth and Design</i> , 2023, 23, 2155-2168.	1.4	4
159	On the potentially transformative role of auxiliary-field quantum Monte Carlo in quantum chemistry: A highly accurate method for transition metals and beyond. <i>Journal of Chemical Physics</i> , 2023, 158, .	1.2	6
160	Comparison of the Performance of Density Functional Methods for the Description of Spin States and Binding Energies of Porphyrins. <i>Molecules</i> , 2023, 28, 3487.	1.7	3
163	Benchmarking Modern Density Functionals for Broad Applications in Chemistry. , 2024, , 78-93.		0
172	Quantum Chemistry of d- and f-Block Elements. , 2024, , 177-192.		1
184	Benchmarks for transition metal spin-state energetics: why and how to employ experimental reference data?. <i>Physical Chemistry Chemical Physics</i> , 2023, 25, 30800-30820.	1.3	0
190	Accessing Ni(0) to Ni(IV) <i>via</i> nickelâ€“carbonâ€“phosphorus bond reorganization. <i>Chemical Communications</i> , 0, , .	2.2	0