# CITATION REPORT List of articles citing

Jacobs ladder of density functional approximations for the exchange-correlation energy

DOI: 10.1063/1.1390175 AIP Conference Proceedings, 2001, , .

Source: https://exaly.com/paper-pdf/32424866/citation-report.pdf

Version: 2024-04-28

This report has been generated based on the citations recorded by exaly.com for the above article. For the latest version of this publication list, visit the link given above.

The third column is the impact factor (IF) of the journal, and the fourth column is the number of citations of the article.

#	Paper	IF	Citations
711	Designing meaningful density functional theory calculations in materials science目 primer. <b>2005</b> , 13, R1-R31		282
710	Local hybrid functionals: an assessment for thermochemical kinetics. <b>2007</b> , 127, 194102		75
709	Double-hybrid functionals for thermochemical kinetics. <b>2008</b> , 112, 3-8		194
708	What can we learn from the adiabatic connection formalism about local hybrid functionals?. <b>2008</b> , 128, 214107		43
707	Validation study of the ability of density functionals to predict the planar-to-three-dimensional structural transition in anionic gold clusters. <b>2009</b> , 131, 064706		66
706	Approximate Density Functionals: Which Should I Choose?. 2009,		14
705	Toward improved density functionals for the correlation energy. <b>2009</b> , 131, 134109		43
704	Performance of ab initio and density functional methods for conformational equilibria of $C(n)H(2n+2)$ alkane isomers (n = 4-8). <b>2009</b> , 113, 11974-83		134
703	Benchmark thermochemistry of the $C(n)H(2n+2)$ alkane isomers ( $n = 2-8$ ) and performance of DFT and composite ab initio methods for dispersion-driven isomeric equilibria. <b>2009</b> , 113, 8434-47		110
702	The distortivity of pi-electrons in conjugated boron rings. <b>2009</b> , 11, 10042-6		3
701	Optimized GGA functional for proton transfer reactions. <b>2009</b> , 113, 14415-9		7
700	DFT Versus the <b>R</b> eal World[[or, Waiting for Godft]). <b>2010</b> , 53, 417-422		21
699	On the performance of eleven DFT functionals in the description of the vibrational properties of aluminosilicates. <b>2010</b> , 110, 406-415		103
698	Performance of 12 DFT functionals in the study of crystal systems: Al2SiO5 orthosilicates and Al hydroxides as a case study. <b>2010</b> , 110, 2260-2273		40
697	An Assessment of Density Functional Methods for Potential Energy Curves of Nonbonded Interactions: The XYG3 and B97-D Approximations. <b>2010</b> , 6, 727-34		86
696	DSD-BLYP: A General Purpose Double Hybrid Density Functional Including Spin Component Scaling and Dispersion Correction (2010, 114, 20801-20808)		261
695	Properties of Carbon Nanotubes: An ab Initio Study Using Large Gaussian Basis Sets and Various DFT Functionals. <b>2011</b> , 115, 8876-8885		41

694	Approximate Density Functionals: Which Should I Choose?. <b>2011</b> ,	3
693	Harmonic electron correlation operator. <b>2011</b> , 135, 034111	1
692	A Parameter-Free Density Functional That Works for Noncovalent Interactions. <b>2011</b> , 2, 983-989	124
691	Nitrogenase structure and function relationships by density functional theory. <b>2011</b> , 766, 267-91	5
690	Investigation of the valence electronic states of Ti(IV) in Ti silicalite-1 coupling X-ray emission spectroscopy and density functional calculations. <b>2011</b> , 13, 19409-19	45
689	An ab initio study of the effect of charge localization on oxygen defect formation and migration energies in magnesium oxide. <b>2011</b> , 467, 2054-2065	26
688	The ab initio calculation of molecular electric, magnetic and geometric properties. <b>2011</b> , 13, 2627-51	55
687	Comparing ab initio density-functional and wave function theories: the impact of correlation on the electronic density and the role of the correlation potential. <b>2011</b> , 135, 114111	36
686	Basis set convergence of explicitly correlated double-hybrid density functional theory calculations. <b>2011</b> , 135, 144119	23
685	Density-functional approaches to noncovalent interactions: a comparison of dispersion corrections (DFT-D), exchange-hole dipole moment (XDM) theory, and specialized functionals. <b>2011</b> , 134, 084107	526
684	W4-11: A high-confidence benchmark dataset for computational thermochemistry derived from first-principles W4 data. <b>2011</b> , 510, 165-178	285
683	Potential-functional embedding theory for molecules and materials. <b>2011</b> , 135, 194104	92
682	Insensitivity of the error of the minimally empirical hybrid functional revTPSSh to its parameters. <b>2012</b> , 137, 224104	1
681	Progress in time-dependent density-functional theory. <b>2012</b> , 63, 287-323	543
680	Perspectives on ab initio molecular simulation of excited-state properties of organic dye molecules in dye-sensitised solar cells. <b>2012</b> , 14, 12044-56	27
679	Accurate Spin-State Energetics of Transition Metal Complexes. 1. CCSD(T), CASPT2, and DFT Study of [M(NCH)6](2+) (M = Fe, Co). <b>2012</b> , 8, 4216-31	115
678	Unraveling the Complexity of Catalytic Reactions via Kinetic Monte Carlo Simulation: Current Status and Frontiers. <b>2012</b> , 2, 2648-2663	158
677	Assessment of theoretical procedures for calculating barrier heights for a diverse set of water-catalyzed proton-transfer reactions. <b>2012</b> , 116, 4211-21	65

676	Comparative Study of Single and Double Hybrid Density Functionals for the Prediction of 3d Transition Metal Thermochemistry. <b>2012</b> , 8, 4102-11	58
675	Libxc: A library of exchange and correlation functionals for density functional theory. <b>2012</b> , 183, 2272-2281	323
674	Exchange-Correlation Functional with Good Accuracy for Both Structural and Energetic Properties while Depending Only on the Density and Its Gradient. <b>2012</b> , 8, 2310-9	232
673	Explicitly correlated benchmark calculations on C8H8 isomer energy separations: how accurate are DFT, double-hybrid, and composite ab initio procedures?. <b>2012</b> , 110, 2477-2491	47
672	First-principles kinetic modeling in heterogeneous catalysis: an industrial perspective on best-practice, gaps and needs. <b>2012</b> , 2, 2010	124
671	Resolution-of-identity approach to Hartree <b>E</b> ock, hybrid density functionals, RPA, MP2 andGWwith numeric atom-centered orbital basis functions. <b>2012</b> , 14, 053020	411
670	The benchmark of Gutzwiller density functional theory in hydrogen systems. <b>2012</b> , 112, 240-246	4
669	Challenges for density functional theory. <b>2012</b> , 112, 289-320	1521
668	Hyper-generalized-gradient functionals constructed from the Lieb-Oxford bound: implementation via local hybrids and thermochemical assessment. <b>2012</b> , 136, 184102	31
667	Assessment of Density Functional Theory for Describing the Correlation Effects on the Ground and Excited State Potential Energy Surfaces of a Retinal Chromophore Model. <b>2013</b> , 9, 3917-32	78
666	Avoiding pitfalls of a theoretical approach: the harmonic oscillator measure of aromaticity index from quantum chemistry calculations. <b>2013</b> , 24, 1171-1184	27
665	Performance of Density Functional Theory for Second Row (4d) Transition Metal Thermochemistry. <b>2013</b> , 9, 3939-46	64
664	Density Functional Theory as a Key Approach in Surface Chemistry and Heterogeneous Catalysis. <b>2013</b> , 405-420	1
663	Spin-component-scaled double hybrids: An extensive search for the best fifth-rung functionals blending DFT and perturbation theory. <b>2013</b> , 34, 2327-44	200
662	Critical Test of Some Computational Chemistry Methods for Prediction of Gas-Phase Acidities and Basicities. <b>2013</b> , 9, 3947-58	31
661	A scalable infrastructure for the performance analysis of passive target synchronization. <b>2013</b> , 39, 132-145	3
660	Assessing the performances of some recently proposed density functionals for the description of organometallic structures. <b>2013</b> , 132, 1	12
659	Implementation of the modified Beckellohnson meta-GGA functional in Quantum Espresso. <b>2013</b> , 184, 1697-1700	12

### (2015-2013)

658	The Becke fuzzy cells integration scheme in the Amsterdam density functional program suite. <b>2013</b> , 34, 1819-27	146
657	First-principles thermodynamic screening approach to photo-catalytic water splitting with co-catalysts. <b>2013</b> , 139, 044710	17
656	A systematic approach to identify cooperatively bound homotrimers. <b>2013</b> , 117, 174-82	15
655	Benchmark Study for the Cysteine-Histidine Proton Transfer Reaction in a Protein Environment: Gas Phase, COSMO, QM/MM Approaches. <b>2013</b> , 9, 1765-77	33
654	Noncollinear density functional theory having proper invariance and local torque properties. <b>2013</b> , 87,	49
653	Halogen Bonds: Benchmarks and Theoretical Analysis. <b>2013</b> , 9, 1918-31	357
652	On the influence of water on the electronic structure of firefly oxyluciferin anions from absorption spectroscopy of bare and monohydrated ions in vacuo. <b>2013</b> , 135, 6485-93	49
651	What can we learn about dispersion from the conformer surface of n-pentane?. 2013, 117, 3118-32	51
650	The melatonin conformer space: benchmark and assessment of wave function and DFT methods for a paradigmatic biological and pharmacological molecule. <b>2013</b> , 117, 2269-77	77
649	A simple DFT-based diagnostic for nondynamical correlation. <b>2013</b> , 132, 1	88
648	C-O bond cleavage of dimethyl ether by transition metal ions: a systematic study on catalytic properties of metals and performance of DFT functionals. <b>2013</b> , 117, 5140-8	21
647	Density Functional Theory in Detail. <b>2013</b> , 127-143	
646	Meta-GGA Exchange-Correlation Functional with a Balanced Treatment of Nonlocality. 2013, 9, 2256-63	53
645	Gradient corrections to the exchange-correlation free energy. <b>2014</b> , 90,	35
644	Cubic-scaling algorithm and self-consistent field for the random-phase approximation with second-order screened exchange. <b>2014</b> , 140, 014107	29
643	Assessment of a Cost-Effective Approach to the Calculation of Kinetic and Thermodynamic Properties of Methyl Methacrylate Homopolymerization: A Comprehensive Theoretical Study. <b>2014</b> , 10, 5668-76	16
642	Appointing silver and bronze standards for noncovalent interactions: a comparison of spin-component-scaled (SCS), explicitly correlated (F12), and specialized wavefunction approaches. <b>2014</b> , 141, 234111	67
641	Computational approaches to homogeneous gold catalysis. <b>2015</b> , 357, 213-83	22

640	Progress on New Approaches to Old Ideas: Orbital-Free Density Functionals. <b>2014</b> , 113-134	23
639	Halogen bonds with benzene: an assessment of DFT functionals. <b>2014</b> , 35, 386-94	65
638	Explicitly correlated coupled cluster benchmarks with realistic-sized ligands for some late-transition metal reactions: basis sets convergence and performance of more approximate methods. <b>2014</b> , 133, 1	33
637	CRYSTAL14: A program for the ab initio investigation of crystalline solids. <b>2014</b> , 114, 1287-1317	1048
636	Conformational equilibria in butane-1,4-diol: a benchmark of a prototypical system with strong intramolecular H-bonds. <b>2014</b> , 118, 293-303	45
635	The interaction of beryllium with benzene and graphene: a comparative investigation based on DFT, MP2, CCSD(T), CAS-SCF and CAS-PT2. <b>2014</b> , 16, 1957-66	10
634	Analytical Energy Gradients in Range-Separated Hybrid Density Functional Theory with Random Phase Approximation. <b>2014</b> , 10, 1968-79	19
633	Novel recipe for double-hybrid density functional computations of linear and nonlinear polarizabilities of molecules and nanoclusters. <b>2014</b> , 118, 5333-42	19
632	A density functional theory study of Na(H2O)n: an example of the impact of self-interaction corrections. <b>2014</b> , 68, 1	11
631	New Benchmark Set of Transition-Metal Coordination Reactions for the Assessment of Density Functionals. <b>2014</b> , 10, 3092-103	142
630	Structural and Vibrational Properties of the Ordered Y2CaGe4O12 Germanate: A Periodic Ab Initio Study. <b>2014</b> , 118, 8090-8101	16
629	Bulk Properties of Transition Metals: A Challenge for the Design of Universal Density Functionals. <b>2014</b> , 10, 3832-9	187
628	Valence to core X-ray emission spectroscopy. <b>2014</b> , 26, 7730-46	72
627	The many faces of halogen bonding: a review of theoretical models and methods. <b>2014</b> , 4, 523-540	163
626	Probing the relationship between spin contamination and first hyperpolarizability: Open-shell MBius anion. <b>2014</b> , 114, 720-724	1
625	Understanding Magnetic Exchange in Molecule-Based Magnets from an Electronic Structure Point of View. <b>2015</b> , 203-246	
624	Anharmonic thermal oscillations of the electron momentum distribution in lithium fluoride. <b>2015</b> , 117, 117402	24
623	Accuracy of Lagrange-sinc functions as a basis set for electronic structure calculations of atoms and molecules. <b>2015</b> , 142, 094116	16

# (2015-2015)

Crystal structure optimisation using an auxiliary equation of state. <b>2015</b> , 143, 184101	15
Fast, accurate evaluation of exact exchange: The occ-RI-K algorithm. <b>2015</b> , 143, 024113	38
Influence of the exchange-correlation functional on the quasi-harmonic lattice dynamics of II-VI semiconductors. <b>2015</b> , 143, 064710	60
Nonadiabatic dynamics with intersystem crossings: A time-dependent density functional theory implementation. <b>2015</b> , 143, 224105	46
Thermodynamics of Passive Film Formation from First Principles. <b>2015</b> , 157-189	2
Piezo-optic tensor of crystals from quantum-mechanical calculations. <b>2015</b> , 143, 144504	19
Electron density analysis of large (molecular and periodic) systems: A parallel implementation. <b>2015</b> , 36, 1940-6	23
London dispersion in molecular chemistryreconsidering steric effects. <b>2015</b> , 54, 12274-96	526
Structure and stability of supramolecular crown ether complexes. <b>2015</b> , 36, 1467-72	5
A simple approximation for the Pauli potential yielding self-consistent electron densities exhibiting proper atomic shell structure. <b>2015</b> , 115, 1629-1634	19
LondonBche Dispersionswechselwirkungen in der Moleklchemie leine Neubetrachtung sterischer Effekte. <b>2015</b> , 127, 12446-12471	170
Global hybrids from the semiclassical atom theory satisfying the local density linear response. <b>2015</b> , 11, 122-31	20
Molecular understandings on the activation of light hydrocarbons over heterogeneous catalysts. <b>2015</b> , 6, 4403-4425	141
Relative energies of water nanoclusters (H2O)20: comparison of empirical and nonempirical double-hybrids with generalized energy-based fragmentation approach. <b>2015</b> , 39, 5534-5539	12
The Nonlocal Correlation Density Functional VV10. <b>2015</b> , 11, 37-102	17
Electrochemical oxidation stability of anions for modern battery electrolytes: a CBS and DFT study. <b>2015</b> , 17, 3697-703	27
Accurate Treatment of Large Supramolecular Complexes by Double-Hybrid Density Functionals Coupled with Nonlocal van der Waals Corrections. <b>2015</b> , 11, 932-9	38
Computation of the Kohn-Sham orbital kinetic energy density in the full-potential linearized augmented plane-wave method. <b>2015</b> , 91,	5
	Fast, accurate evaluation of exact exchange: The occ-RI-K algorithm. 2015, 143, 024113  Influence of the exchange-correlation functional on the quasi-harmonic lattice dynamics of II-VI semiconductors. 2015, 143, 064710  Nonadiabatic dynamics with intersystem crossings: A time-dependent density functional theory implementation. 2015, 143, 224105  Thermodynamics of Passive Film Formation from First Principles. 2015, 157-189  Piezo-optic tensor of crystals from quantum-mechanical calculations. 2015, 143, 144504  Electron density analysis of large (molecular and periodic) systems: A parallel implementation. 2015, 36, 1940-6  London dispersion in molecular chemistry-reconsidering steric effects. 2015, 54, 12274-96  Structure and stability of supramolecular crown ether complexes. 2015, 36, 1467-72  A simple approximation for the Pauli potential yielding self-consistent electron densities exhibiting proper atomic shell structure. 2015, 115, 1629-1634  London&che Dispersionswechselwirkungen in der Molek@chemie @ine Neubetrachtung sterischer Effekte. 2015, 127, 12446-12471  Global hybrids from the semiclassical atom theory satisfying the local density linear response. 2015, 11, 122-31  Molecular understandings on the activation of light hydrocarbons over heterogeneous catalysts. 2015, 6, 4403-4425  Relative energies of water nanoclusters (H2O)20: comparison of empirical and nonempirical double-hybrids with generalized energy-based fragmentation approach. 2015, 39, 5534-5539  The Nonlocal Correlation Density Functional VV10. 2015, 11, 37-102  Electrochemical oxidation stability of anions for modern battery electrolytes: a CBS and DFT study. 2015, 17, 3697-703  Accurate Treatment of Large Supramolecular Complexes by Double-Hybrid Density Functionals Coupled with Nonlocal van der Waals Corrections. 2015, 11, 932-9  Computation of the Kohn-Sham orbital kinetic energy density in the full-potential linearized

604	On the DFT ground state of crystalline bromine and iodine. <b>2015</b> , 16, 728-32	14
603	Direct and indirect effects of dispersion interactions on the electric properties of weakly bound complexes. <b>2015</b> , 119, 3112-24	11
602	Reaction barrier heights for cycloreversion of heterocyclic rings: An Achilles heel for DFT and standard ab initio procedures. <b>2015</b> , 458, 1-8	51
601	Choosing a density functional for static molecular polarizabilities. <b>2015</b> , 635, 257-261	34
600	Reformulation of the D3(Becke-Johnson) Dispersion Correction without Resorting to Higher than CIDispersion Coefficients. <b>2015</b> , 11, 3163-70	51
599	Designing a paradigm for parameter-free double-hybrid density functionals through the adiabatic connection path. <b>2015</b> , 134, 1	22
598	Reliable Prediction with Tuned Range-Separated Functionals of the Singlet-Triplet Gap in Organic Emitters for Thermally Activated Delayed Fluorescence. <b>2015</b> , 11, 3851-8	256
597	Is It Possible To Obtain Coupled Cluster Quality Energies at near Density Functional Theory Cost? Domain-Based Local Pair Natural Orbital Coupled Cluster vs Modern Density Functional Theory. <b>2015</b> , 11, 4054-63	184
596	Frank Discussion of the Status of Ground-State Orbital-Free DFT. <b>2015</b> , 71, 221-245	32
595	Real-space grids and the Octopus code as tools for the development of new simulation approaches for electronic systems. <b>2015</b> , 17, 31371-96	276
594	The nature of the bonding in symmetrical pincer palladacycles. <b>2015</b> , 44, 7570-7	12
593	DFT: A Theory Full of Holes?. <b>2015</b> , 66, 283-304	111
592	Electronic-structure-based material descriptors: (in)dependence on self-interaction and Hartree-Fock exchange. <b>2015</b> , 51, 5602-5	17
591	Using computational chemistry to design Ru photosensitizers with directional charge transfer. <b>2015</b> , 304-305, 146-165	48
590	The Nature of the Interlayer Interaction in Bulk and Few-Layer Phosphorus. 2015, 15, 8170-5	205
589	Assessment of the TCA functional in computational chemistry and solid-state physics. <b>2015</b> , 134, 1	8
588	Structural and elastic anisotropy of crystals at high pressures and temperatures from quantum mechanical methods: The case of Mg2SiO4 forsterite. <b>2015</b> , 142, 204502	28
587	Performance of a Non-Local van der Waals Density Functional on the Dissociation of H2 on Metal Surfaces. <b>2015</b> , 119, 12146-58	37

# (2016-2015)

586	Quantum chemical benchmark study on 46 RNA backbone families using a dinucleotide unit. <b>2015</b> , 11, 4972-91	74
585	Modeling thermochemical reactions in thermal energy storage systems. <b>2015</b> , 375-415	6
584	Computational Isotope Geochemistry. <b>2016</b> , 12, 117-156	1
583	Order of stabilities in water nanoclusters: Insight from some recent double-hybrid functionals. <b>2016</b> , 116, 1173-1178	
582	Diastereoselective Synthesis of and Mechanistic Understanding for the Formation of 2-Piperidinones from Imines and Cyano-Substituted Anhydrides. <b>2016</b> , 22, 4794-801	15
581	Assessing the Accuracy of Across-the-Scale Methods for Predicting Carbohydrate Conformational Energies for the Examples of Glucose and Emaltose. <b>2016</b> , 12, 6157-6168	66
580	Self-consistent implementation of meta-GGA functionals for the ONETEP linear-scaling electronic structure package. <b>2016</b> , 145, 204114	11
579	Towards quantifying the role of exact exchange in the prediction hydrogen bond spin-spin coupling constants involving fluorine. <b>2016</b> , 145, 084301	8
578	Random phase approximation with second-order screened exchange for current-carrying atomic states. <b>2016</b> , 145, 224106	8
577	Rungs 1 to 4 of DFT Jacob's ladder: Extensive test on the lattice constant, bulk modulus, and cohesive energy of solids. <b>2016</b> , 144, 204120	142
576	Validation of local hybrid functionals for TDDFT calculations of electronic excitation energies. <b>2016</b> , 144, 074106	93
575	Unexpected cold curve sensitivity to GGA exchange form. <b>2016</b> , 135, 1	
574	Nonequilibrium solvent effects in Born-Oppenheimer molecular dynamics for ground and excited electronic states. <b>2016</b> , 144, 154104	7
573	A dataset of highly accurate homolytic N?Br bond dissociation energies obtained by Means of W2 theory. <b>2016</b> , 116, 52-60	22
572	Bond breaking in stretched molecules: multi-reference methods versus density functional theory. <b>2016</b> , 135, 1	17
57 <sup>1</sup>	How Much Can Density Functional Approximations (DFA) Fail? The Extreme Case of the FeO4 Species. <b>2016</b> , 12, 1525-33	26
570	Choosing an appropriate model chemistry in a big data context: Application to dative bonding. <b>2016</b> , 1085, 46-55	1
569	Magnetic properties with multiwavelets and DFT: the complete basis set limit achieved. <b>2016</b> , 18, 21145-61	29

568	Effect of the Exchange-Correlation Potential on the Transferability of Brfisted-Evans-Polanyi Relationships in Heterogeneous Catalysis. <b>2016</b> , 12, 2121-6	15
567	Patching the Exchange-Correlation Potential in Density Functional Theory. <b>2016</b> , 12, 2224-33	6
566	Seeking for Spin-Opposite-Scaled Double-Hybrid Models Free of Fitted Parameters. <b>2016</b> , 120, 3726-30	20
565	The nature of inter- and intramolecular interactions in F2OXe(IHX (X= F, Cl, Br, I) complexes. <b>2016</b> , 22, 119	O
564	Density Functional Theory Methods for Computing and Predicting Mechanical Properties. <b>2016</b> , 131-158	
563	Encyclopedia of Geochemistry. <b>2016</b> , 1-7	O
562	Logros y perspectivas de la Quthica Te町ca. <b>2016</b> , 27, 278-285	
561	Exchange-Correlation Catastrophe in Cu-Au: A Challenge for Semilocal Density Functional Approximations. <b>2016</b> , 117, 066401	11
560	General approach for band gap calculation of semiconductors and insulators. <b>2016</b> , 213, 2834-2837	6
559	Solution of the KohnBham equations for many-electron atoms confined by penetrable walls. <b>2016</b> , 135, 1	18
558	Accurate Kohn-Sham ionization potentials from scaled-opposite-spin second-order optimized effective potential methods. <b>2016</b> , 37, 2081-90	21
557	Kinetic-energy-density dependent semilocal exchange-correlation functionals. <b>2016</b> , 116, 1641-1694	62
556	Assessing exchange-correlation functional performance for structure and property predictions of oxyfluoride compounds from first principles. <b>2016</b> , 94,	22
555	Assessment of quantum chemical methods for the calculation of homolytic NB bond dissociation energies. <b>2016</b> , 5-6, 28-35	4
554	Overview of Electronic Structure Methods. <b>2016</b> , 39-66	2
553	Toward the Computational Prediction of Muon Sites and Interaction Parameters. <b>2016</b> , 85, 091014	19
552	Extending the density functional embedding theory to finite temperature and an efficient iterative method for solving for embedding potentials. <b>2016</b> , 144, 124106	9
551	First principles optimally tuned range-separated density functional theory for prediction of phosphorus-hydrogen spin-spin coupling constants. <b>2016</b> , 18, 18431-40	17

### (2017-2016)

550	[PW12O40]3EA systematical study with different functionals of density functional theory. <b>2016</b> , 1089, 28-34	8
549	Improving B3LYP heats of formation with three-dimensional molecular descriptors. <b>2016</b> , 37, 1175-90	8
548	Dielectric Matrix Formulation of Correlation Energies in the Random Phase Approximation: Inclusion of Exchange Effects. <b>2016</b> , 12, 2191-202	27
547	The S66x8 benchmark for noncovalent interactions revisited: explicitly correlated ab initio methods and density functional theory. <b>2016</b> , 18, 20905-25	127
546	What Are the Ground State Structures of C20 and C24? An Explicitly Correlated Ab Initio Approach. <b>2016</b> , 120, 153-60	32
545	Benchmark ab Initio Conformational Energies for the Proteinogenic Amino Acids through Explicitly Correlated Methods. Assessment of Density Functional Methods. <b>2016</b> , 12, 444-54	75
544	Can DFT and ab initio methods describe all aspects of the potential energy surface of cycloreversion reactions?. <b>2016</b> , 114, 21-33	18
543	A conundrum for density functional theory. <b>2017</b> , 355, 28-29	56
542	Atomistic Modeling-Based Design of Novel Materials . <b>2017</b> , 19, 1600688	10
54 <sup>1</sup>	Directions for Use of Density Functional Theory: A Short Instruction Manual for Chemists. <b>2017</b> , 225-267	1
540	Simulation study on the effects of chemical structure and molecular size on the acceptor strength in poly(3-hexylthiophene)-based copolymer with alternating donor and acceptor for photovoltaic applications. <b>2017</b> , 50, 065502	1
539	Development of New Density Functional Approximations. <b>2017</b> , 68, 155-182	32
538	Can X-ray constrained Hartree-Fock wavefunctions retrieve electron correlation?. 2017, 4, 136-146	35
537	Vanishing-Overhead Linear-Scaling Random Phase Approximation by Cholesky Decomposition and an Attenuated Coulomb-Metric. <b>2017</b> , 13, 1647-1655	32
536	Benchmarking density functionals in conjunction with Grimme's dispersion correction for noble gas dimers (Ne2, Ar2, Kr2, Xe2, Rn2). <b>2017</b> , 117, e25358	23
535	Correlation effects on the interelectronic distributions of localized electron pairs. 2017, 136, 1	1
534	Assessing DFT-D3 Damping Functions Across Widely Used Density Functionals: Can We Do Better?. <b>2017</b> , 13, 2043-2052	48
533	Machine Learning, Quantum Chemistry, and Chemical Space. <b>2017</b> , 225-256	41

532	What Makes a Density Functional Approximation Good? Insights from the Left Fukui Function. <b>2017</b> , 13, 2373-2377	26
531	Is the Accuracy of Density Functional Theory for Atomization Energies and Densities in Bonding Regions Correlated?. <b>2017</b> , 8, 2076-2081	51
530	Exchange functionals based on finite uniform electron gases. <b>2017</b> , 146, 114108	11
529	Efficient Computation of Exchange Energy Density with Gaussian Basis Functions. <b>2017</b> , 13, 2571-2580	15
528	Accurate Intermolecular Potential for the C Dimer: The Performance of Different Levels of Quantum Theory. <b>2017</b> , 13, 274-285	14
527	First-Principles Prediction of a Stable Hexagonal Phase of CH3NH3PbI3. <b>2017</b> , 29, 6003-6011	40
526	Shedding Light on the Accuracy of Optimally Tuned Range-Separated Approximations for Evaluating Oxidation Potentials. <b>2017</b> , 121, 4189-4201	9
525	Gauging the performance of some density functionals including dispersion and nonlocal corrections for relative energies of water 20-mers. <b>2017</b> , 75, 132-136	3
524	Dissecting the accountability of parameterized and parameter-free single-hybrid and double-hybrid functionals for photophysical properties of TADF-based OLEDs. <b>2017</b> , 146, 234304	16
523	Conventional and Explicitly Correlated ab Initio Benchmark Study on Water Clusters: Revision of the BEGDB and WATER27 Data Sets. <b>2017</b> , 13, 3136-3152	65
522	Can DFT and ab initio methods adequately describe binding energies in strongly interacting C6X6?C2Xn Leomplexes?. <b>2017</b> , 493, 12-19	1
521	Practical principles of density functional theory for catalytic reaction simulations on metal surfaces [from theory to applications. <b>2017</b> , 43, 861-885	13
520	Laplacian-dependent models of the kinetic energy density: Applications in subsystem density functional theory with meta-generalized gradient approximation functionals. <b>2017</b> , 146, 064105	36
519	Performance of wave function and density functional methods for water hydrogen bond spin-spin coupling constants. <b>2017</b> , 23, 134	2
518	The Elephant in the Room of Density Functional Theory Calculations. 2017, 8, 1449-1457	60
517	Random-Phase Approximation Methods. <b>2017</b> , 68, 421-445	80
516	Reference Determinant Dependence of the Random Phase Approximation in 3d Transition Metal Chemistry. <b>2017</b> , 13, 100-109	13
515	Accurate Dissociation of Chemical Bonds Using DFT-in-DFT Embedding Theory with External Orbital Orthogonality. <b>2017</b> , 121, 256-264	15

514	Metal Ion Modeling Using Classical Mechanics. <b>2017</b> , 117, 1564-1686	189
513	Structure of Chemisorbed CO(2) Species in Amine-Functionalized Mesoporous Silicas Studied by Solid-State NMR and Computer Modeling. <b>2017</b> , 139, 389-408	75
512	Ab initio theory and modeling of water. <b>2017</b> , 114, 10846-10851	246
511	Evaluation of the Factors Impacting the Accuracy of C NMR Chemical Shift Predictions using Density Functional Theory-The Advantage of Long-Range Corrected Functionals. <b>2017</b> , 13, 5798-5819	49
510	Electrochemical phase diagrams of Ni from ab initio simulations: role of exchange interactions on accuracy. <b>2017</b> , 29, 475501	10
509	Interpolative Separable Density Fitting Decomposition for Accelerating Hybrid Density Functional Calculations with Applications to Defects in Silicon. <b>2017</b> , 13, 5420-5431	29
508	Metalligand Bifunctional Catalysis: The AcceptedlMechanism, the Issue of Concertedness, and the Function of the Ligand in Catalytic Cycles Involving Hydrogen Atoms. <b>2017</b> , 7, 6635-6655	176
507	Challenges for semilocal density functionals with asymptotically nonvanishing potentials. 2017, 96,	12
506	The parameter uncertainty inflation fallacy. <b>2017</b> , 147, 104102	21
505	Electron Density Errors and Density-Driven Exchange-Correlation Energy Errors in Approximate Density Functional Calculations. <b>2017</b> , 13, 4753-4764	33
504	Comparative Study of Nonhybrid Density Functional Approximations for the Prediction of 3d Transition Metal Thermochemistry. <b>2017</b> , 13, 4907-4913	25
503	Assessing the ability of DFT methods to describe static electron correlation effects: CO core level binding energies as a representative case. <b>2017</b> , 147, 024106	8
502	Assessment of Tuned Range Separated Exchange Functionals for Spectroscopies and Properties of Uranium Complexes. <b>2017</b> , 13, 3614-3625	13
501	Bias-Free Chemically Diverse Test Sets from Machine Learning. <b>2017</b> , 19, 544-554	6
500	Accurate potential energy surfaces for hydrogen abstraction reactions: A benchmark study on the XYG3 doubly hybrid density functional. <b>2017</b> , 38, 2326-2334	3
499	Assessing Excited State Energy Gaps with Time-Dependent Density Functional Theory on Ru(II) Complexes. <b>2017</b> , 13, 4123-4145	33
498	SBH10: A Benchmark Database of Barrier Heights on Transition Metal Surfaces. <b>2017</b> , 121, 19807-19815	67
497	Seeking an accurate generalized-gradient approximation functional for high pressure molecular fluids. <b>2017</b> , 122, 185902	6

496	Computational Plasmonics: Numerical Techniques. <b>2017</b> , 341-368	1
495	On the opposite-spin to same-spin ratio of absolute and interaction MP2 correlation energy in parameter-free spin-opposite-scaled double hybrids. <b>2017</b> , 684, 423-426	9
494	Characterization of Thin Film Materials using SCAN meta-GGA, an Accurate Nonempirical Density Functional. <b>2017</b> , 7, 44766	41
493	Stability of the chlorinated derivatives of the DNA/RNA nucleobases, purine and pyrimidine toward radical formation via homolytic C?Cl bond dissociation. <b>2017</b> , 117, e25319	5
492	A simple model for the Slater exchange potential and its performance for solids. <b>2017</b> , 117, 40-47	17
491	Challenges in large scale quantum mechanical calculations. <b>2017</b> , 7, e1290	65
490	Directly patching high-level exchange-correlation potential based on fully determined optimized effective potentials. <b>2017</b> , 147, 244111	1
489	Exact functionals for correlated electronphoton systems. <b>2017</b> , 19, 113036	15
488	Chemi- and Bioluminescence of Cyclic Peroxides. <b>2018</b> , 118, 6927-6974	172
487	Simplified DFT methods for consistent structures and energies of large systems. <b>2018</b> , 30, 213001	28
486	Application of a Coulomb energy density functional for atomic nuclei: Case studies of local density approximation and generalized gradient approximation. <b>2018</b> , 97,	6
485	Dipole moments of molecules with multi-reference character from optimally tuned range-separated density functional theory. <b>2018</b> , 39, 1508-1516	9
484	Impact of long-range electrostatic and dispersive interactions on theoretical predictions of adsorption and catalysis in zeolites. <b>2018</b> , 312, 51-65	22
483	Electronic Exchange and Correlation in van der Waals Systems: Balancing Semilocal and Nonlocal Energy Contributions. <b>2018</b> , 14, 1361-1369	20
482	How reliable are Minnesota density functionals for modeling phosphorusBydrogen NMR spinBpin coupling constants?. <b>2018</b> , 137, 1	1
481	Rational Density Functional Selection Using Game Theory. <b>2018</b> , 58, 61-67	15
480	Predicting Optical Properties from Ab Initio Calculations. 2018, 83-104	
	Accurate critical pressures for structural phase transitions of group IV, III-V, and II-VI compounds	

478	Relative stability of FeS2 polymorphs with the random phase approximation approach. <b>2018</b> , 6, 6606-6616	18
477	Long-range corrected density functional through the density matrix expansion based semilocal exchange hole. <b>2018</b> , 20, 8991-8998	17
476	Quantum modeling of ultrafast photoinduced charge separation. <b>2018</b> , 30, 013002	20
475	Jacob's Ladder as Sketched by Escher: Assessing the Performance of Broadly Used Density Functionals on Transition Metal Surface Properties. <b>2018</b> , 14, 395-403	44
474	Chemically driven surface effects in polar intermetallic topological insulators ABi. 2018, 20, 26372-26385	3
473	An efficient first principles method for molecular pump-probe NEXAFS spectra: Application to thymine and azobenzene. <b>2018</b> , 149, 144112	16
472	Prototyping Ultrafast Charge Separation by Means of Time-Dependent Density Functional Methods. <b>2018</b> , 1-19	
471	Heavy nuclei: Introduction to density functional theory and variations on the theme?. <b>2018</b> , 133, 1	2
470	Reaction energetics of hydrogen on Si(100) surface: A periodic many-electron theory study. <b>2018</b> , 149, 244105	6
469	Computational screening of methylammonium based halide perovskites with bandgaps suitable for perovskite-perovskite tandem solar cells. <b>2018</b> , 149, 214701	10
468	Efficient lattice constants and energy bandgaps for condensed systems from a meta-GGA level screened range-separated hybrid functional. <b>2018</b> , 149, 094105	10
467	The Nonlocal Kernel in van der Waals Density Functionals as an Additive Correction: An Extensive Analysis with Special Emphasis on the B97M-V and B97M-V Approaches. 2018, 14, 5725-5738	95
466	A local tensor that unifies kinetic energy density and vorticity in density functional theory. <b>2018</b> , 144109	5
465	Embedded Cluster Density Approximation for Exchange-Correlation Energy: A Natural Extension of the Local Density Approximation. <b>2018</b> , 14, 6211-6225	8
464	Error-Controlled Exploration of Chemical Reaction Networks with Gaussian Processes. <b>2018</b> , 14, 5238-5248	51
463	A systematic electronic structure study of the OD bond dissociation energy of hydrogen peroxide and the electron affinity of the hydroxyl radical. <b>2018</b> , 137, 1	5
462	From one to three, exploring the rungs of Jacob⊠ ladder in magnetic alloys. <b>2018</b> , 91, 1	11
461	Exploring conformational preferences of alanine tetrapeptide by CCSD(T), MP2, and dispersion-corrected DFT methods. <b>2018</b> , 702, 69-75	6

460	Chemical Bond Energies of 3d Transition Metals Studied by Density Functional Theory. <b>2018</b> , 14, 3479-3492	39
459	A Comprehensive Assessment of the Effectiveness of Orbital Optimization in Double-Hybrid Density Functionals in the Treatment of Thermochemistry, Kinetics, and Noncovalent Interactions. <b>2018</b> , 122, 5610-5624	16
458	Benchmarking DFT methods on linear and nonlinear electric properties of spatially confined molecules. <b>2018</b> , 118, e25666	11
457	Assessment of Density Functional Methods for Geometry Optimization of Bimolecular van der Waals Complexes. <b>2018</b> , 14, 3004-3013	17
456	Density Functional Theory under the Bubbles and Cube Numerical Framework. <b>2018</b> , 14, 4237-4245	3
455	Computational screening and molecular design of anthracene-based semiconductors. <b>2018</b> , 61, 87-95	4
454	Semi-empirical or non-empirical double-hybrid density functionals: which are more robust?. <b>2018</b> , 20, 23175-23194	68
453	Calibrating the Extended Hākel Method to Quantitatively Screen the Electronic Properties of Materials. <b>2018</b> , 8, 10530	1
452	Bond-breaking excitations with diverging coupling matrix of response density functional theory from highest-level functionals. <b>2018</b> , 91, 1	0
451	Efficient and Accurate Prediction of Nuclear Magnetic Resonance Shielding Tensors with Double-Hybrid Density Functional Theory. <b>2018</b> , 14, 4756-4771	40
450	Assessing the performance of the Tao-Mo semilocal density functional in the projector-augmented-wave method. <b>2018</b> , 149, 044120	32
449	Shannon Entropy in Atoms: A Test for the Assessment of Density Functionals in Kohn-Sham Theory. <b>2018</b> , 6, 36	4
448	Torsional Potentials of Glyoxal, Oxalyl Halides, and Their Thiocarbonyl Derivatives: Challenges for Popular Density Functional Approximations. <b>2018</b> , 14, 4806-4817	7
447	Density functional theory versus quantum Monte Carlo simulations of Fermi gases in the optical-lattice arena. <b>2018</b> , 91, 1	1
446	Communication: xDH double hybrid functionals can be qualitatively incorrect for non-equilibrium geometries: Dipole moment inversion and barriers to radical-radical association using XYG3 and XYGJ-OS. <b>2018</b> , 148, 171102	17
445	Theoretical Models for Bimetallic Surfaces and Nanoalloys. <b>2018</b> , 23-60	1
444	Ab Initio Finite Temperature Auxiliary Field Quantum Monte Carlo. 2018, 14, 4722-4732	31
443	Accurate computation of X-ray absorption spectra with ionization potential optimized global hybrid functional. <b>2018</b> , 149, 064111	15

442	A Systematic Protocol for Benchmarking Guest-Host Interactions by First-Principles Computations: Capturing CO in Clathrate Hydrates. <b>2018</b> , 24, 9353-9363	9
441	Predicting vapor liquid equilibria using density functional theory: A case study of argon. <b>2018</b> , 148, 224501	8
440	Neural-network Kohn-Sham exchange-correlation potential and its out-of-training transferability. <b>2018</b> , 148, 241737	38
439	Local hybrid functionals: Theory, implementation, and performance of an emerging new tool in quantum chemistry and beyond. <b>2019</b> , 9, e1378	60
438	Quantum Chemical and QM/MM Models in Biochemistry. <b>2019</b> , 2022, 75-104	3
437	Statistically representative databases for density functional theory via data science. <b>2019</b> , 21, 19092-19103	13
436	Laplacian free and asymptotic corrected semilocal exchange potential applied to the band gap of solids. <b>2019</b> , 21, 19639-19650	14
435	Adsorption on transition metal surfaces: Transferability and accuracy of DFT using the ADS41 dataset. <b>2019</b> , 100,	30
434	Oganesson ist ein Halbleiter: Ber die relativitische Bandl©kenkontraktion in den schwersten Edelgasen. <b>2019</b> , 131, 14398-14402	8
433	Toward a Quantum-Chemical Benchmark Set for Enzymatically Catalyzed Reactions: Important Steps and Insights. <b>2019</b> , 123, 7057-7074	12
432	Large-Scale Benchmark of Exchange-Correlation Functionals for the Determination of Electronic Band Gaps of Solids. <b>2019</b> , 15, 5069-5079	92
431	<b>B</b> 2PLYP and <b>B</b> 2GPPLYP: The First Two Double-Hybrid Density Functionals with Long-Range Correction Optimized for Excitation Energies. <b>2019</b> , 15, 4735-4744	55
430	Oganesson Is a Semiconductor: On the Relativistic Band-Gap Narrowing in the Heaviest Noble-Gas Solids. <b>2019</b> , 58, 14260-14264	18
429	First-Principles Investigation of Spin-Phonon Coupling in Vanadium-Based Molecular Spin Quantum Bits. <b>2019</b> , 58, 10260-10268	31
428	Low-order many-body interactions determine the local structure of liquid water. <b>2019</b> , 10, 8211-8218	29
427	Off-the-shelf DFT-DISPersion methods: Are they now "on-trend" for organic molecular crystals?. <b>2019</b> , 151, 044106	5
426	Toward a Specific Reaction Parameter Density Functional for H2 + Ni(111): Comparison of Theory with Molecular Beam Sticking Experiments. <b>2019</b> , 123, 20420-20433	9
425	A Benchmark of Density Functional Approximations For Thermochemistry and Kinetics of Hydride Reductions of Cyclohexanones. <b>2019</b> , 8, 788-806	3

424	Machine Learning the Physical Nonlocal Exchange-Correlation Functional of Density-Functional Theory. <b>2019</b> , 10, 6425-6431	34
423	The Reliability of the Density-Functional Theory in Actinide Endohedral Systems. <b>2019</b> , 2, 1900138	4
422	Restoring the iso-orbital limit of the kinetic energy density in relativistic density functional theory. <b>2019</b> , 151, 174114	5
421	Adventures in DFT by a wavefunction theorist. <b>2019</b> , 151, 160901	16
420	Toward the Exact Exchange-Correlation Potential: A Three-Dimensional Convolutional Neural Network Construct. <b>2019</b> , 10, 7264-7269	22
419	Density Functional Analysis: The Theory of Density-Corrected DFT. <b>2019</b> , 15, 6636-6646	35
418	Range-separation and the multiple radii functional approximation inspired by the strongly interacting limit of density functional theory. <b>2019</b> , 151, 184101	5
417	Force balance approach for advanced approximations in density functional theories. <b>2019</b> , 151, 154107	4
416	Effect of the meso/beta halogenation in the photoelectronic properties and aromaticity of expanded porphyrins. <b>2019</b> , 385, 112052	5
415	Localizing electron density errors in density functional theory. <b>2019</b> , 21, 20927-20938	7
414	Thermal Decomposition of Hydroxylammonium Nitrate: ReaxFF Training Set Development for Molecular Dynamics Simulations. <b>2019</b> ,	1
413	Calculation of Free-Energy Barriers with TD-DFT: A Case Study on Excited-State Proton Transfer in Indigo. <b>2019</b> , 123, 8485-8495	11
412	Semilocal exchange-correlation potentials for solid-state calculations: Current status and future directions. <b>2019</b> , 126, 110902	21
411	The influence of antenna and anchoring moieties on the improvement of photoelectronic properties in Zn(ii)-porphyrin-TiO as potential dye-sensitized solar cells. <b>2019</b> , 21, 4339-4348	12
410	Reliable electrochemical phase diagrams of magnetic transition metals and related compounds from high-throughput ab initio calculations. <b>2019</b> , 3,	18
409	Are Explicit Solvent Models More Accurate than Implicit Solvent Models? A Case Study on the Menschutkin Reaction. <b>2019</b> , 123, 5580-5589	17
408	Minimally Empirical Double-Hybrid Functionals Trained against the GMTKN55 Database: revDSD-PBEP86-D4, revDOD-PBE-D4, and DOD-SCAN-D4. <b>2019</b> , 123, 5129-5143	128
407	Fundamental Role of Fock Exchange in Relativistic Density Functional Theory. <b>2019</b> , 10, 3580-3585	11

406	Numerical methods for KohnBham density functional theory. <b>2019</b> , 28, 405-539	10
405	Density Functionals from the Multiple-Radii Approach: Analysis and Recovery of the Kinetic Correlation Energy. <b>2019</b> , 15, 3580-3590	4
404	A Density-Based Basis-Set Correction for Wave Function Theory. <b>2019</b> , 10, 2931-2937	18
403	Long-range screened hybrid-functional theory satisfying the local-density linear response. <b>2019</b> , 99,	10
402	The Metal Hydride Problem of Computational Chemistry: Origins and Consequences. <b>2019</b> , 123, 2888-2900	13
401	Advances in Sustainable Catalysis: A Computational Perspective. <b>2019</b> , 7, 182	27
400	Nature of Halide-Water Interactions: Insights from Many-Body Representations and Density Functional Theory. <b>2019</b> , 15, 2983-2995	17
399	Well-behaved versus ill-behaved density functionals for single bond dissociation: Separating success from disaster functional by functional for stretched H. <b>2019</b> , 150, 094115	18
398	Functional-renormalization-group aided density functional analysis for the correlation energy of the two-dimensional homogeneous electron gas. <b>2019</b> , 99,	8
397	Improved DFT Adsorption Energies with Semiempirical Dispersion Corrections. <b>2019</b> , 15, 3250-3259	29
396	van der Waals exchange-correlation functionals over bulk and surface properties of transition metals. <b>2019</b> , 31, 315501	7
395	The Lowest-Energy Isomer of C2Si2H4 Is a Bridged Ring: Reinterpretation of the Spectroscopic Data Based on DFT and Coupled-Cluster Calculations. <b>2019</b> , 7, 51	
394	A quantum chemical study of the effect of substituents in governing the strength of the SE bonds of sulfenyl-type fluorides toward homolytic dissociation and fluorine atom transfer. <b>2019</b> , 20, 100186	2
393	First-Principles Methods in the Investigation of the Chemical and Transport Properties of Materials under Extreme Conditions. <b>2019</b> , 5, 421-433	3
392	Formation of small clusters of NaCl dihydrate in the gas phase. <b>2019</b> , 43, 4342-4348	10
391	Remarkable Structural Effect on the Gold-Hydrogen Analogy in Hydrogen-Doped Gold Cluster. <b>2019</b> , 123, 1973-1982	2
390	From DFT to machine learning: recent approaches to materials science review. <b>2019</b> , 2, 032001	206
389	A Trip to the Density Functional Theory Zoo: Warnings and Recommendations for the User. <b>2019</b> , 72, 563	77

388	Improvement of functionals in density functional theory by the inverse KohnBham method and density functional perturbation theory. <b>2019</b> , 52, 245003	8
387	Dispersion-driven conformational preference in the gas phase: Microwave spectroscopic and theoretical study of allyl isocyanate. <b>2019</b> , 151, 194304	5
386	Ethylene adsorption on Ag(111), Rh(111) and Ir(111) by (meta)-GGA based density functional theory calculations. <b>2019</b> , 32, 437-443	5
385	Adiabatic connection in density functional theory in two-dimensions: A semi-analytic wavefunction based study for two-electron atomic systems. <b>2019</b> , 151, 204104	O
384	A step in the direction of resolving the paradox of Perdew-Zunger self-interaction correction. <b>2019</b> , 151, 214108	34
383	Density functional theory-based investigations of solute kinetics and precipitate formation in binary magnesium-rare earth alloys: A review. <b>2019</b> , 159, 235-256	11
382	Photophysics of OLED Materials with Emitters Exhibiting Thermally Activated Delayed Fluorescence and Used in Hole/Electron Transporting Layer from Optimally Tuned Range-Separated Density Functional Theory. <b>2019</b> , 123, 746-761	11
381	Phonon properties and thermal conductivity from first principles, lattice dynamics, and the Boltzmann transport equation. <b>2019</b> , 125, 011101	82
380	Challenges in Modeling Electrochemical Reaction Energetics with Polarizable Continuum Models. <b>2019</b> , 9, 920-931	100
379	Triplet Tuning: A Novel Family of Non-Empirical Exchange-Correlation Functionals. <b>2019</b> , 15, 1226-1241	23
378	Investigation of the Exchange-Correlation Potentials of Functionals Based on the Adiabatic Connection Interpolation. <b>2019</b> , 15, 1006-1015	16
377	Performance of DFT for C Isomerization Energies: A Noticeable Exception to Jacob's Ladder. <b>2019</b> , 123, 257-266	13
376	Hydrogen bonding networks in gabapentin protic pharmaceutical salts: NMR and in silico studies. <b>2019</b> , 57, 243-255	1
375	Investigations of Stacked DNA Base-Pair Steps: Highly Accurate Stacking Interaction Energies, Energy Decomposition, and Many-Body Stacking Effects. <b>2019</b> , 15, 95-115	39
374	Ab initio dielectric response function of diamond and other relevant high pressure phases of carbon. <b>2020</b> , 32, 095401	9
373	Simulations and Materials Chemistry in the Age of Big Data. <b>2020</b> , 60, 452-459	18
372	Ambipolar Resistive Switching in an Ultrathin Surface-Supported Metal-Organic Framework Vertical Heterojunction. <b>2020</b> , 20, 1080-1088	29
371	The local density approximation in density functional theory. <b>2020</b> , 2, 35-73	9

# (2020-2020)

370	Vibrational Response of Felodipine in the THz Domain: Optical and Neutron Spectroscopy Versus Plane-Wave DFT Modeling. <b>2020</b> , 41, 1301-1336	5
369	Layered Cathode Materials for Lithium-Ion Batteries: Review of Computational Studies on LiNi1如CoxMnyO2 and LiNi1如CoxAlyO2. <b>2020</b> , 32, 915-952	76
368	Empirical Double-Hybrid Density Functional Theory: A Third Waylin Between WFT and DFT. <b>2020</b> , 60, 787-804	71
367	Conformational preferences of cationic theptide in water studied by CCSD(T), MP2, and DFT methods. <b>2020</b> , 6, e04721	3
366	Computational chemistry approaches for the preparation of supported catalysts: Progress and challenges. <b>2020</b> , 391, 539-547	5
365	A Local Hybrid Functional with Wide Applicability and Good Balance between (De)Localization and Left-Right Correlation. <b>2020</b> , 16, 5645-5657	18
364	Measuring Density-Driven Errors Using Kohn-Sham Inversion. <b>2020</b> , 16, 5014-5023	9
363	The CECAM electronic structure library and the modular software development paradigm. <b>2020</b> , 153, 024117	5
362	Double-Hybrid DFT Functionals for the Condensed Phase: Gaussian and Plane Waves Implementation and Evaluation. <b>2020</b> , 25,	6
361	Pyrroles and Their Benzo Derivatives: Structure. <b>2020</b> ,	
360	The Fermi-Ltwdin self-interaction correction for ionization energies of organic molecules. <b>2020</b> , 153, 184303	9
359	Efficient Calculation of Small Molecule Binding in Metal <b>D</b> rganic Frameworks and Porous Organic Cages. <b>2020</b> , 124, 27529-27541	13
358	Concluding remarks for the new horizons in density functional theory Faraday Discussion. <b>2020</b> , 224, 509-514	1
357	Spin-Crossover from a Well-Behaved, Low-Cost meta-GGA Density Functional. <b>2020</b> , 124, 9889-9894	7
356	Theoretical analysis of an anion-Lomplex: IC6F6. <b>2020</b> , 33, 285-290	1
355	Assessing the effect of regularization on the molecular properties predicted by SCAN and self-interaction corrected SCAN meta-GGA. <b>2020</b> , 22, 18060-18070	1
354	Double-hybrid density functional theory for g-tensor calculations using gauge including atomic orbitals. <b>2020</b> , 153, 054105	5
	Applications of Quantum Chemistry in Pharmaceutical Process Development: Current State and	8

352	Machine learning accurate exchange and correlation functionals of the electronic density. <b>2020</b> , 11, 3509	55
351	Exchange-correlation functionals for band gaps of solids: benchmark, reparametrization and machine learning. <b>2020</b> , 6,	63
350	Snakes on the Rungs of Jacob's Ladder: Anomalous Vibrational Spectra from Double-Hybrid DFT Methods. <b>2020</b> , 124, 6899-6902	1
349	Exact exchange-correlation potential of effectively interacting Kohn-Sham systems. <b>2020</b> , 101,	1
348	Decomplexation as a rate limitation in the thiol-Michael addition of N-acrylamides. 2020, 18, 6364-6377	3
347	Study of self-interaction errors in density functional predictions of dipole polarizabilities and ionization energies of water clusters using Perdew-Zunger and locally scaled self-interaction corrected methods. <b>2020</b> , 153, 164304	14
346	Structural, mechanical, electronic properties of refractory HfAl intermetallics from SCAN meta-GGA density functional calculations. <b>2020</b> , 254, 123423	3
345	DFT-D4 counterparts of leading meta-generalized-gradient approximation and hybrid density functionals for energetics and geometries. <b>2020</b> , 41, 2562-2572	17
344	Large Impact of Approximate Exchange-Correlation Functionals on Modeling the Water Gas Shift Reaction on Copper. <b>2020</b> , 124, 22506-22520	3
343	Isotope effects in x-ray absorption spectra of liquid water. <b>2020</b> , 102,	4
343	Isotope effects in x-ray absorption spectra of liquid water. <b>2020</b> , 102,  Preface. <b>2020</b> , xix-xxiii	4
		4
342	Preface. <b>2020</b> , xix-xxiii	4
34 <sup>2</sup> 34 <sup>1</sup>	Preface. 2020, xix-xxiii Introduction. 2020, 1-14	4
34 <sup>2</sup> 34 <sup>1</sup> 34 <sup>0</sup>	Preface. 2020, xix-xxiii  Introduction. 2020, 1-14  Overview. 2020, 15-59	4
34 <sup>2</sup> 34 <sup>1</sup> 34 <sup>0</sup>	Preface. 2020, xix-xxiii  Introduction. 2020, 1-14  Overview. 2020, 15-59  Theoretical Background. 2020, 60-80	4
34 <sup>2</sup> 34 <sup>1</sup> 34 <sup>0</sup> 339	Preface. 2020, xix-xxiii  Introduction. 2020, 1-14  Overview. 2020, 15-59  Theoretical Background. 2020, 60-80  Periodic Solids and Electron Bands. 2020, 81-108	4

### (2020-2020)

334	Functionals for Exchange and Correlation I. <b>2020</b> , 171-187
333	Functionals for Exchange and Correlation II. <b>2020</b> , 188-214
332	Electronic Structure of Atoms. <b>2020</b> , 215-229
331	Pseudopotentials. <b>2020</b> , 230-258
330	Overview of Chapters 1218. <b>2020</b> , 259-261
329	Plane Waves and Grids: Basics. <b>2020</b> , 262-282
328	Plane Waves and Real-Space Methods: Full Calculations. <b>2020</b> , 283-294
327	Localized Orbitals: Tight-Binding. <b>2020</b> , 295-319
326	Localized Orbitals: Full Calculations. <b>2020</b> , 320-331
325	Augmented Functions: APW, KKR, MTO. <b>2020</b> , 332-364
324	Augmented Functions: Linear Methods. <b>2020</b> , 365-385
323	Locality and Linear-Scaling O(N) Methods. <b>2020</b> , 386-410
322	Quantum Molecular Dynamics (QMD). <b>2020</b> , 411-426
321	Response Functions: Phonons and Magnons. <b>2020</b> , 427-445
320	Excitation Spectra and Optical Properties. <b>2020</b> , 446-464
319	Surfaces, Interfaces, and Lower-Dimensional Systems. <b>2020</b> , 465-480
318	Wannier Functions. <b>2020</b> , 481-498
317	Polarization, Localization, and Berry Phases. <b>2020</b> , 499-516

316	Topology of the Electronic Structure of a Crystal: Introduction. <b>2020</b> , 517-530
315	Two-Band Models: Berry Phase, Winding, and Topology. <b>2020</b> , 531-546
314	Topological Insulators I: Two Dimensions. <b>2020</b> , 547-568
313	Topological Insulators II: Three Dimensions. <b>2020</b> , 569-580
312	Functional Equations. <b>2020</b> , 581-583
311	LSDA and GGA Functionals. <b>2020</b> , 584-586
310	Adiabatic Approximation. <b>2020</b> , 587-589
309	Perturbation Theory, Response Functions, and Green Functions. <b>2020</b> , 590-599
308	Dielectric Functions and Optical Properties. <b>2020</b> , 600-606
307	Coulomb Interactions in Extended Systems. <b>2020</b> , 607-619
306	Stress from Electronic Structure. <b>2020</b> , 620-626
305	Energy and Stress Densities. <b>2020</b> , 627-636
304	Alternative Force Expressions. <b>2020</b> , 637-643
303	Scattering and Phase Shifts. <b>2020</b> , 644-646
302	Useful Relations and Formulas. <b>2020</b> , 647-650
301	Numerical Methods. <b>2020</b> , 651-660
300	Iterative Methods in Electronic Structure. <b>2020</b> , 661-676
299	Two-Center Matrix Elements: Expressions for Arbitrary Angular Momentum l. <b>2020</b> , 677-685

298 Dirac Equation and SpinDrbit Interaction. **2020**, 686-696

297	Berry Phase, Curvature, and Chern Numbers. <b>2020</b> , 697-700	
296	Quantum Hall Effect and Edge Conductivity. <b>2020</b> , 701-703	
295	Index. <b>2020</b> , 756-762	
294	Evaluation of Local Hybrid Functionals for Electric Properties: Dipole Moments and Static and Dynamic Polarizabilities. <b>2020</b> , 124, 8346-8358	6
293	Accurate Hybrid Density Functionals with UW12 Correlation. <b>2020</b> , 16, 6176-6194	5
292	Efficient yet accurate dispersion-corrected semilocal exchange-correlation functionals for non-covalent interactions. <b>2020</b> , 153, 084117	8
291	Toward universal substituent constants: Model chemistry sensitivity of descriptors from the quantum theory of atoms in molecules. <b>2020</b> , 41, 2485-2503	1
290	Small data materials design with machine learning: When the average model knows best. <b>2020</b> , 128, 054901	9
289	Mean-field density matrix decompositions. <b>2020</b> , 153, 214109	4
288	Machine-learned electron correlation model based on frozen core approximation. <b>2020</b> , 153, 184108	4
287	Ensemble Density Functional Theory: Insight from the Fluctuation-Dissipation Theorem. <b>2020</b> , 125, 233001	9
286	Halogen Bond of Halonium Ions: Benchmarking DFT Methods for the Description of NMR Chemical Shifts. <b>2020</b> , 16, 7690-7701	4
285	Improved solid stability from a screened range-separated hybrid functional by satisfying semiclassical atom theory and local density linear response. <b>2020</b> , 102,	7
284	The one-electron self-interaction error in 74 density functional approximations: a case study on hydrogenic mono- and dinuclear systems. <b>2020</b> , 22, 15805-15830	16
283	The ONETEP linear-scaling density functional theory program. <b>2020</b> , 152, 174111	45
282	Completing density functional theory by machine learning hidden messages from molecules. <b>2020</b> , 6,	59
281	TURBOMOLE: Modular program suite for ab initio quantum-chemical and condensed-matter simulations. <b>2020</b> , 152, 184107	255

280	Canonical and DLPNO-Based G4(MP2)XK-Inspired Composite Wave Function Methods Parametrized against Large and Chemically Diverse Training Sets: Are They More Accurate and/or Robust than Double-Hybrid DFT?. <b>2020</b> , 16, 4238-4255	19
279	The CRYSTAL code, 1976-2020 and beyond, a long story. <b>2020</b> , 152, 204111	61
278	CP2K: An electronic structure and molecular dynamics software package - Quickstep: Efficient and accurate electronic structure calculations. <b>2020</b> , 152, 194103	421
277	Exact Generalized Kohn-Sham Theory for Hybrid Functionals. <b>2020</b> , 10,	10
276	Carbon Isotope Fractionation of Substituted Benzene Analogs during Oxidation with Ozone and Hydroxyl Radicals: How Should Experimental Data Be Interpreted?. <b>2020</b> , 54, 6713-6722	3
275	Improvements in the orbitalwise scaling down of Perdew-Zunger self-interaction correction in many-electron regions. <b>2020</b> , 152, 174112	17
274	Plane wave basis set correction methods for RPA correlation energies. <b>2020</b> , 152, 134103	5
273	TurboRVB: A many-body toolkit for ab initio electronic simulations by quantum Monte Carlo. <b>2020</b> , 152, 204121	19
272	Principal interacting orbital: A chemically intuitive method for deciphering bonding interaction. <b>2020</b> , 10, e1469	19
271	An Overview of Self-Consistent Field Calculations Within Finite Basis Sets. <b>2020</b> , 25,	16
270	Noncovalent Quantum Machine Learning Corrections to Density Functionals. <b>2020</b> , 16, 2647-2653	13
269	Thermochemistry of FeOH Species: Assessment of Some DFT Functionals. <b>2020</b> , 16, 2430-2435	4
268	Implications of the fractional charge of hydroxide at the electrochemical interface. <b>2020</b> , 22, 6964-6969	5
267	Molecular Structure and Modeling of Water-Air and Ice-Air Interfaces Monitored by Sum-Frequency Generation. <b>2020</b> , 120, 3633-3667	43
266	TD-DFT spin-adiabats with analytic nonadiabatic derivative couplings. <b>2020</b> , 152, 044112	7
265	The devil in the details: A tutorial review on some undervalued aspects of density functional theory calculations. <b>2020</b> , 120, e26332	28
264	Dealing with Spin States in Computational Organometallic Catalysis. <b>2020</b> , 191-226	5
263	Relativistic local hybrid functionals and their impact on 1s core orbital energies. <b>2020</b> , 152, 214103	4

262	Adsorption and activation of CO on Zr ( $n = 2-7$ ) clusters. <b>2020</b> , 22, 16877-16886	5
261	Piecewise linearity, freedom from self-interaction, and a Coulomb asymptotic potential: three related yet inequivalent properties of the exact density functional. <b>2020</b> , 22, 16467-16481	16
260	Benchmarking of DFT methods using experimental free energies and volumes of activation for the cycloaddition of alkynes to cuboidal Mo3S4 clusters. <b>2020</b> , 120, e26353	2
259	Substituted -Benzynes: Properties of the Triple Bond. <b>2020</b> , 85, 9905-9914	2
258	Assessment of SAPT(DFT) with meta-GGA functionals. <b>2020</b> , 26, 102	3
257	Performance of DFT functionals for properties of small molecules containing beryllium, tungsten and hydrogen. <b>2020</b> , 22, 100731	3
256	Difficulties of Popular Density Functionals to Describe the Conformational Isomerism in Iodoacetic Acid. <b>2020</b> , 124, 5570-5579	2
255	Using electronegativity and hardness to test density functionals. <b>2020</b> , 152, 244113	2
254	Projector Augmented Wave Method with Gauss-Type Atomic Orbital Basis: Implementation of the Generalized Gradient Approximation and Mesh Grid Quadrature. <b>2020</b> , 16, 4883-4898	1
253	State-Targeted Energy Projection: A Simple and Robust Approach to Orbital Relaxation of Non-Aufbau Self-Consistent Field Solutions. <b>2020</b> , 16, 5067-5082	39
252	Competing excited-state deactivation processes in bacteriophytochromes. <b>2020</b> , 243-268	1
251	Finding the optimal exchange-correlation functional to describe the excited state properties of push-pull organic dyes designed for thermally activated delayed fluorescence. <b>2020</b> , 22, 16387-16399	11
250	In silico Raman spectroscopy of YAlO single-crystalline film. <b>2020</b> , 231, 118111	3
249	Performance of Electronic Structure Methods for the Description of Hākel-M <b>B</b> ius Interconversions in Extended Bystems. <b>2020</b> , 124, 2380-2397	11
248	WIEN2k: An APW+lo program for calculating the properties of solids. <b>2020</b> , 152, 074101	408
247	Quasi-degenerate states and their dynamics in oxygen deficient reducible metal oxides. <b>2020</b> , 152, 050901	12
246	Calculation of Diamagnetic Susceptibility Tensors of Organic Crystals: From Coronene to Pharmaceutical Polymorphs. <b>2020</b> , 124, 1409-1420	4
245	How accurate are approximate quantum chemical methods at modelling solute-solvent interactions in solvated clusters?. <b>2020</b> , 22, 3855-3866	13

244	Range-Separated Density-Functional Theory in Combination with the Random Phase Approximation: An Accuracy Benchmark. <b>2020</b> , 16, 2985-2994	8
243	Accurate computed spin-state energetics for Co(iii) complexes: implications for modelling homogeneous catalysis. <b>2020</b> , 49, 6478-6487	11
242	How accurate are TD-DFT excited-state geometries compared to DFT ground-state geometries?. <b>2020</b> , 41, 1718-1729	25
241	Nuclear density functional theory. <b>2020</b> , 5, 1740061	6
240	Double hybrid DFT calculations with Slater type orbitals. <b>2020</b> , 41, 1660-1684	10
239	Hybrid functionals with system-dependent parameters: Conceptual foundations and methodological developments. <b>2020</b> , 10, e1476	6
238	Ion Pairing and Multiple Ion Binding in Calcium Carbonate Solutions Based on a Polarizable AMOEBA Force Field and Ab Initio Molecular Dynamics. <b>2020</b> , 124, 3568-3582	12
237	The Trip to the Density Functional Theory Zoo Continues: Making a Case for Time-Dependent Double Hybrids for Excited-State Problems. <b>2021</b> , 74, 3	23
236	Fitting elephants in the density functionals zoo: Statistical criteria for the evaluation of density functional theory methods as a suitable replacement for counting parameters. <b>2021</b> , 121, e26379	3
235	Modeling thermochemical reactions in thermal energy storage systems. <b>2021</b> , 497-542	1
234	Comprehensive Benchmark Study on the Calculation of Si NMR Chemical Shifts. <b>2021</b> , 60, 272-285	9
233	Benchmarking DFT Calculations of 1H and 13C Chemical Shifts in Monosubstituted Ferrocenes. <b>2021</b> , 121, e26456	2
232	Local self-interaction correction method with a simple scaling factor. <b>2021</b> , 23, 2406-2418	9
231	Climbing to the Top of Mount Fuji: Uniting Theory and Observations of Oxygen Triple Isotope Systematics. <b>2021</b> , 86, 97-135	4
230	Critical benchmarking of popular composite thermochemistry models and density functional approximations on a probabilistically pruned benchmark dataset of formation enthalpies. <b>2021</b> , 154, 044113	5
229	Electronic and geometric determinants of adsorption: fundamentals and applications. <b>2021</b> , 3, 022001	6
228	Performance of SCAN Meta-GGA Functionals on Nonlinear Mechanics of Graphene-Like g-SiC. <b>2021</b> , 11, 120	
227	Meta-Local Density Functionals: A New Rung on Jacob's Ladder. <b>2021</b> , 17, 943-948	O

### (2021-2021)

226	Advancing photoreforming of organics: highlights on photocatalyst and system designs for selective oxidation reactions. <b>2021</b> , 14, 1140-1175	33
225	Picture-change correction in relativistic density functional theory. <b>2021</b> , 23, 15458-15474	1
224	Replacing hybrid density functional theory: motivation and recent advances. <b>2021</b> , 50, 8470-8495	23
223	Ab initio construction of the energy density functional for electron systems with the functional-renormalization-group-aided density functional theory. <b>2021</b> , 3,	4
222	Computationally Guided Searches for Efficient Catalysts through Chemical/Materials Space: Progress and Outlook. <b>2021</b> , 125, 6495-6507	2
221	Effect of the Current Dependence of Tau-Dependent Exchange-Correlation Functionals on Nuclear Shielding Calculations. <b>2021</b> , 17, 1469-1479	7
220	Metal Sulfide Nanoparticle Synthesis with Ionic Liquids - State of the Art and Future Perspectives. <b>2021</b> , 10, 272-295	3
219	rSCAN-D4: Dispersion corrected meta-generalized gradient approximation for general chemical applications. <b>2021</b> , 154, 061101	22
218	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. <b>2021</b> , 154, 074109	9
217	Correct Structural Phase Stability of FeS2, TiO2, and MnO2 from a Semilocal Density Functional. <b>2021</b> , 125, 4284-4291	4
216	Reduction of Hartree-Fock Wavefunctions to Kohn-Sham Effective Potentials Using Multiresolution Analysis. <b>2021</b> , 17, 1408-1420	1
215	Implementation of Perdew-Zunger self-interaction correction in real space using Fermi-LWdin orbitals. <b>2021</b> , 154, 084112	4
214	Describing adsorption of benzene, thiophene, and xenon on coinage metals by using the Zaremba-Kohn theory-based model. <b>2021</b> , 154, 124705	1
213	Ensemble generalized Kohn-Sham theory: The good, the bad, and the ugly. <b>2021</b> , 154, 094125	8
212	Adsorption and Activation of CO on Small-Sized Cu-Zr Bimetallic Clusters. 2021, 125, 2558-2572	8
211	Static dipole polarizabilities of polyacenes using self-interaction-corrected density functional approximations. <b>2021</b> , 154, 114305	5
210	Exploring and enhancing the accuracy of interior-scaled Perdew-Zunger self-interaction correction. <b>2021</b> , 154, 094105	5
209	Implementation and Validation of Local Hybrid Functionals with Calibrated Exchange-Energy Densities for Nuclear Shielding Constants. <b>2021</b> , 125, 2697-2707	3

208 Computational Methods in Organometallic Chemistry. **2021**, 19-49

207	A promising Zn-Ti layered double hydroxide/Fe-bearing montmorillonite composite as an efficient photocatalyst for Cr(VI) reduction: Insight into the role of Fe impurity in montmorillonite. <b>2021</b> , 546, 148835	13
206	Theoretical Prediction of Two-Dimensional Materials, Behavior, and Properties. <b>2021</b> , 15, 5959-5976	8
205	CHAL336 Benchmark Set: How Well Do Quantum-Chemical Methods Describe Chalcogen-Bonding Interactions?. <b>2021</b> , 17, 2783-2806	18
204	Concepts, models, and methods in computational heterogeneous catalysis illustrated through CO2 conversion. <b>2021</b> , 11, e1530	11
203	The best density functional theory functional for the prediction of H and C chemical shifts of protonated alkylpyrroles. <b>2021</b> , 42, 1248-1262	2
202	Exploring Avenues beyond Revised DSD Functionals: II. Random-Phase Approximation and Scaled MP3 Corrections. <b>2021</b> , 125, 4628-4638	10
201	Assessment of Performance of Density Functionals for Predicting Potential Energy Curves in Hydrogen Storage Applications. <b>2021</b> , 125, 4245-4257	O
200	Exploring Avenues beyond Revised DSD Functionals: I. Range Separation, with DSD as a Special Case. <b>2021</b> , 125, 4614-4627	15
199	Lessons learned from first-principles calculations of transition metal oxides. <b>2021</b> , 154, 174704	5
198	On the Use of Normalized Metrics for Density Sensitivity Analysis in DFT. <b>2021</b> , 125, 4639-4652	3
197	Analysis of Recent BLYP- and PBE-Based Range-Separated Double-Hybrid Density Functional Approximations for Main-Group Thermochemistry, Kinetics, and Noncovalent Interactions. <b>2021</b> , 125, 4026-4035	8
196	Theoretical Study of Electronic Structure of Charged Fullerenes. <b>2021</b> , 2021, 1-10	
195	Sensitivity of the Fermi surface to the treatment of exchange and correlation. <b>2021</b> , 103,	1
194	Spin-Opposite-Scaled Range-Separated Exchange Double-Hybrid Models (SOS-RSX-DHs): Marriage Between DH and RSX/SOS-RSX Is Not Always a Happy Match. <b>2021</b> , 17, 4077-4091	2
193	Toward a First-Principles Framework for Predicting Collective Properties of Electrolytes. <b>2021</b> , 54, 2833-2843	14
192	Assessing locally range-separated hybrid functionals from a gradient expansion of the exchange energy density. <b>2021</b> , 154, 214101	2
191	Crystal Structure Prediction Methods for Organic Molecules: State of the Art. <b>2021</b> , 12, 593-623	5

190	Decomposed Mean-Field Simulations of Local Properties in Condensed Phases. <b>2021</b> , 12, 6048-6055	3
189	Combining Machine Learning and Computational Chemistry for Predictive Insights Into Chemical Systems. <b>2021</b> , 121, 9816-9872	53
188	Investigating functional performance and substituent effect in modelling molecular structure, UV-visible spectra, and optical properties of D-FA conjugated organic dye molecules: a DFT and TD-DFT study. <b>2021</b> , 27, 229	1
187	Multilevel approach to the initial guess for self-consistent field calculations. e26782	1
186	Quasi-dimensional models applied to kinetic and exchange energy density functionals. <b>2021</b> , 94, 1	
185	Predicting the substituent effects in the optical and electrochemical properties of N,N'-substituted isoindigos. <b>2021</b> , 20, 927-938	1
184	Accurate density functional made more versatile. <b>2021</b> , 155, 024103	3
183	Density Functional Geometries and Zero-Point Energies in Ab Initio Thermochemical Treatments of Compounds with First-Row Atoms (H, C, N, O, F). <b>2021</b> , 17, 4872-4890	6
182	Solving the strong-correlation problem in materials. <b>2021</b> , 44, 597	0
181	Nuclear Quantum Effect and Its Temperature Dependence in Liquid Water from Random Phase Approximation via Artificial Neural Network. <b>2021</b> , 12, 6354-6362	3
180	Software for the frontiers of quantum chemistry: An overview of developments in the Q-Chem 5 package. <b>2021</b> , 155, 084801	115
179	Nuclear energy density functionals grounded in ab initio calculations. <b>2021</b> , 104,	2
178	A Statistically Supported Antioxidant Activity DFT Benchmark-The Effects of Hartree-Fock Exchange and Basis Set Selection on Accuracy and Resources Uptake. <b>2021</b> , 26,	3
177	Tailoring the Gibbs Free Energy of the Nitroxide Exchange Reaction: Substituent and Solvent Effects. <b>2021</b> , 125, 7616-7624	1
176	Predictive optical photoabsorption of AgAu(DMBT) via efficient TDDFT simulations. 2021, 155, 084103	2
175	Assessing Density Functional Theory for Chemically Relevant Open-Shell Transition Metal Reactions. <b>2021</b> , 17, 6134-6151	19
174	The relevance of electronic perturbations in the warm dense electron gas. <b>2021</b> , 155, 124116	8
173	Surprisingly Good Performance of XYG3 Family Functionals Using a Scaled KS-MP3 Correlation. <b>2021</b> , 12, 9368-9376	2

172	Simulating electronic excitation and dynamics with real-time propagation approach to TDDFT within plane-wave pseudopotential formulation. <b>2021</b> , 155, 100901	3
171	Accurate Prediction of Band Structure of FeS: A Hard Quest of Advanced First-Principles Approaches. <b>2021</b> , 9, 747972	
170	Modeling Liquid Water by Climbing up Jacob's Ladder in Density Functional Theory Facilitated by Using Deep Neural Network Potentials. <b>2021</b> , 125, 11444-11456	13
169	Coupled Cluster Benchmark of New DFT and Local Correlation Methods: Mechanisms of Hydroarylation and Oxidative Coupling Catalyzed by Ru(II, III) Chloride Carbonyls. <b>2021</b> , 125, 8987-8999	6
168	Bandgap of two-dimensional materials: Thorough assessment of modern exchange-correlation functionals. <b>2021</b> , 155, 104103	4
167	Forecasting System of Computational Time of DFT/TDDFT Calculations under the Multiverse Ansatz via Machine Learning and Cheminformatics. <b>2021</b> , 6, 2001-2024	3
166	Pure non-local machine-learned density functional theory for electron correlation. 2021, 12, 344	15
165	Application-Specific Fault Tolerance via Data Access Characterization. <b>2011</b> , 340-352	2
164	A DFT and wave function theory study of hydrogen adsorption on small beryllium oxide clusters. <b>2020</b> , 139, 1	2
163	Electronic Structure: Basic Theory and Practical Methods. <b>2020</b> ,	38
162	Toward a Resolution of the Static Correlation Problem in Density Functional Theory from Semidefinite Programming. <b>2021</b> , 12, 385-391	6
161	Climbing Jacob's Ladder of Structural Refinement: Introduction of a Localized Molecular Orbital-Based Embedding for Accurate X-ray Determinations of Hydrogen Atom Positions. <b>2021</b> , 12, 463-471	13
160	Screening methods for linear-scaling short-range hybrid calculations on CPU and GPU architectures. <b>2017</b> , 146, 144108	5
159	Screened range-separated hybrid by balancing the compact and slowly varying density regimes: Satisfaction of local density linear response. <b>2020</b> , 152, 044111	11
158	Unveiling the role of short-range exact-like exchange in the optimally tuned range-separated hybrids for fluorescence lifetime modeling. <b>2020</b> , 152, 204301	3
157	The Hubbard-U correction and optical properties of d metal oxide photocatalysts. <b>2020</b> , 153, 224116	5
156	Climbing Jacob ladder: A density functional theory case study for Ag2ZnSnSe4 and Cu2ZnSnSe4. <b>2021</b> , 3, 015002	4
155	Performance of the strongly constrained and appropriately normed density functional for solid-state materials. <b>2018</b> , 2,	106

154	Achieving accurate energetics beyond (semi-)local density functional theory: Illustrated with transition metal disulfides, Cu2ZnSnS4, and Na3PS4 related semiconductors. <b>2019</b> , 3,	4
153	Nonlocal van der Waals functionals for solids: Choosing an appropriate one. <b>2019</b> , 3,	41
152	Design and analysis of machine learning exchange-correlation functionals via rotationally invariant convolutional descriptors. <b>2019</b> , 3,	29
151	Nonlocal exchange and correlation energy functionals using the Yukawa potential as ingredient: Application to the linear response of the uniform electron gas. <b>2021</b> , 104,	
150	Performance of new exchangeBorrelation functionals in providing vertical excitation energies of metal complexes. <b>2021</b> , 140, 1	О
149	Do Double-Hybrid Exchange-Correlation Functionals Provide Accurate Chemical Shifts? A Benchmark Assessment for Proton NMR. <b>2021</b> , 17, 6876-6885	9
148	A simple DFT-based diagnostic for nondynamical correlation. <b>2014</b> , 251-259	
147	Non-local Exchange and Correlation. <b>2015</b> , 163-195	
146	Encyclopedia of Geochemistry. <b>2018</b> , 347-352	
145	Density-gradient-free variable in exchange-correlation functionals for detecting inhomogeneities in the electron density. <b>2018</b> , 2,	
144	Paramagnetic NMR Shielding Tensors and Ring Currents: Efficient Implementation and Application to Heavy Element Compounds. <b>2021</b> , 125, 9707-9723	5
143	Practical treatment of singlet oxygen with density-functional theory and the multiplet-sum method. <b>2021</b> , 140, 1	1
142	Prototyping Ultrafast Charge Separation by Means of Time-Dependent Density Functional Methods. <b>2020</b> , 325-343	
141	Recent Developments in Density Functional Approximations. <b>2020</b> , 213-226	2
140	Singlet fission relevant energetics from optimally tuned range-separated hybrids. <b>2020</b> , 22, 27060-27076	2
139	Machine learning the derivative discontinuity of density-functional theory.	1
138	Elevating density functional theory to chemical accuracy for water simulations through a density-corrected many-body formalism. <b>2021</b> , 12, 6359	9
137	Three decades of unveiling the complex chemistry of C-nitroso species with computational chemistry.	1

136	Improved electronic structure prediction of chalcopyrite semiconductors from a semilocal density functional based on Pauli kinetic energy enhancement factor. <b>2021</b> , 34,	
135	Extended Benchmark Set of Main-Group Nuclear Shielding Constants and NMR Chemical Shifts and Its Use to Evaluate Modern DFT Methods. <b>2021</b> ,	6
134	Readdressing molecular dissociation within the KohnBham formalism of density-functional theory: simple models and a different point of view.	
133	Estimation of electron absorption spectra and lifetime of the two lowest singlet excited states of pyrimidine nucleobases and their derivatives. <b>2021</b> , 1250, 131863	2
132	O2 on Ag(110): A puzzle for exchange-correlation functionals. <b>2021</b> , 554, 111424	
131	Role of Computational Science in Materials and Systems Design for Sustainable Energy Applications: An Industry Perspective. 1	
130	Heisenberg Spin Hamiltonian Derived from a Multiple Grand Canonical Spin Density Functional Theory with a Principal Nonlocal Exchangellorrelation Energy Functional. <b>2022</b> , 91,	
129	Efficient basis sets for core-excited states motivated by Slater's rules 2022,	2
128	Operando Characterization of Organic Mixed Ionic/Electronic Conducting Materials 2022,	4
127	Proton Affinity Values of Fentanyl and Fentanyl Analogues Pertinent to Ambient Ionization and Detection <b>2022</b> ,	O
126	Determination of length scale parameters of strain gradient continuum theory for crystalline solids using a computational quantum mechanical model based on density functional theory. <b>2022</b> , 36, 97-104	2
125	Double-hybrid density functionals for the condensed phase: Gradients, stress tensor, and auxiliary-density matrix method acceleration <b>2022</b> , 156, 074107	1
124	Electronic excitations through the prism of mean-field decomposition techniques 2022, 156, 061101	1
123	Construction of meta-GGA functionals through restoration of exact constraint adherence to regularized SCAN functionals <b>2022</b> , 156, 034109	5
122	Review of computational approaches to predict the thermodynamic stability of inorganic solids.	1
121	Density Functional Theory Transformed into a One-Electron Reduced-Density-Matrix Functional Theory for the Capture of Static Correlation <b>2022</b> , 1382-1388	О
120	Barriers to predictive high-throughput screening for spin-crossover. <b>2022</b> , 206, 111161	1
119	Hyperfine Coupling Constants in Local Exact Two-Component Theory 2021,	3

118	Molecular Simulations of Aqueous Electrolytes: Role of Explicit Inclusion of Charge Transfer into Force Fields. <b>2021</b> , 125, 13069-13076	2
117	Density Functional Theory for Transition Metal Catalysis. 2022,	
116	Excited-state properties of organic semiconductor dyes as electrically pumped lasing candidates from new optimally tuned range-separated models <b>2022</b> ,	1
115	The duhka of DFT: a noble path to better functionals via a point electron approximation for the exchange $\Box$ or relation hole $\Box$ $\Box$ <b>2022</b> ,	Ο
114	Benchmark Study on the Calculation of Sn NMR Chemical Shifts <b>2022</b> , 61, 3903-3917	1
113	Quasi-Relativistic Calculation of EPR Tensors with Derivatives of the Decoupling Transformation, Gauge-Including Atomic Orbitals, and Magnetic Balance <b>2022</b> ,	2
112	Study of Self-Interaction Errors in Density Functional Calculations of Magnetic Exchange Coupling Constants Using Three Self-Interaction Correction Methods <b>2022</b> ,	2
111	EPR Spectroscopy of Cu(II) Complexes: Prediction of g-Tensors Using Double-Hybrid Density Functional Theory. <b>2022</b> , 8, 36	Ο
110	Mechanism of Interlayer Transport on a Growing Au(111) Surface: 2D vs. 3D Growth. <b>2022</b> , 101944	0
109	Dispersion corrected rSCAN based global hybrid functionals: rSCANh, rSCAN0, and rSCAN50 <b>2022</b> , 156, 134105	4
108	Optimal Tuning Perspective of Range-Separated Double Hybrid Functionals <b>2022</b> , 18, 2331-2340	1
107	Impact of Intrinsic Density Functional Theory Errors on the Predictive Power of Nitrogen Cycle Electrocatalysis Models <b>2022</b> , 12, 4784-4791	4
106	Pure and Hybrid SCAN, rSCAN, and rSCAN: Which One Is Preferred in KS- and HF-DFT Calculations, and How Does D4 Dispersion Correction Affect This Ranking?. <b>2021</b> , 27,	2
105	Molecule-Specific Uncertainty Quantification in Quantum Chemical Studies. 2022, 62,	3
104	Systematic Evaluation of Modern Density Functional Methods for the Computation of NMR Shifts of 3d Transition-Metal Nuclei <b>2021</b> ,	0
103	Atomistic modeling of Li- and post-Li-ion batteries. <b>2022</b> , 6,	1
102	Chemical Information. <b>2022</b> , 349-374	
101	Double Hybrids and Noncovalent Interactions: How Far Can We Go?. 2022,	1

100	Do Double-Hybrid Functionals Benefit from Regularization in the PT2 Term? Observations from an Extensive Benchmark <b>2022</b> , 3499-3506	3
99	First-principles derivation and properties of density-functional average-atom models. <b>2022</b> , 4,	2
98	Accurate Prediction of Nuclear Magnetic Resonance Parameters via the XYG3 Type of Doubly Hybrid Density Functionals <b>2022</b> ,	1
97	Designing 3d metal oxides: selecting optimal density functionals for strongly correlated materials <b>2022</b> ,	O
96	Data-driven and constrained optimization of semi-local exchange and nonlocal correlation functionals for materials and surface chemistry <b>2022</b> ,	1
95	Quantum Chemical Approaches to the Calculation of NMR Parameters: From Fundamentals to Recent Advances. <b>2022</b> , 8, 50	3
94	A theoretical investigation of nonlinear optical and electronic molecular parameters of hexabutyloxytryphenylene and halogenated hexabutyloxytryphenylene molecules using density functional theory (DFT) for nonlinear device applications. <b>2022</b> , 97, 065808	1
93	Electronic band structure and chemical bonding in trigonal Se and Te. <b>2022</b> , 12, 055110	
92	Assessment of XC functionals for the study of organic molecules with superhalogen substitution. A systematic comparison between DFT and CCSD(T) <b>2022</b> , 156, 184303	O
91	Many-body effects in the X-ray absorption spectra of liquid water <b>2022</b> , 119, e2201258119	3
90	Comparative Study of Vibrational Raman Optical Activity with Different Time-Dependent Density Functional Approximations: The VROA36 Database <b>2022</b> , 126, 2909-2927	1
89	A Combined Machine Learning and High-Energy X-ray Diffraction Approach to Understanding Liquid and Amorphous Metal Oxides. <b>2022</b> , 91,	O
88	Assessing Recent Time-Dependent Double-Hybrid Density Functionals on Doublet <b>D</b> oublet Excitations.	1
87	Conformational Energy Benchmark for Longer n-Alkane Chains.	2
86	Electronic structure of oxide and halide perovskites. 2022,	
85	Analytic Gradients for the Long-Range-Corrected XYG3 Type of Doubly Hybrid Density Functionals: Theory, Implementation, and Assessment. <b>2022</b> , 126, 3937-3946	
84	Comparative density functional studies of BiMO3 polymorphs ( $M = Al$ , $Ga$ , $In$ ) based on LDA, $GGA$ , and meta- $GGA$ functionals.	0
83	A Local Hybrid Exchange Functional Approximation from First Principles.	3

82	Exploiting Ligand Additivity for Transferable Machine Learning of Multireference Character across Known Transition Metal Complex Ligands.	Ο
81	Gold⊞ydrogen Analogy in SmallBized HydrogenDoped Gold Clusters Revisited.	
80	Fullerenes Pose a Strain on Hybrid Density Functional Theory. <b>2022</b> , 126, 4709-4720	3
79	Recent Advances in Cartesian-Grid DFT in Atoms and Molecules. 10,	
78	Surrogate- and invariance-boosted contrastive learning for data-scarce applications in science. <b>2022</b> , 13,	O
77	Uniting Nonempirical and Empirical Density Functional Approximation Strategies Using Constraint-Based Regularization. <b>2022</b> , 13, 6896-6904	Ο
76	Benchmarking time-dependent density functional theory for singlet excited states of thermally activated delayed fluorescence chromophores. <b>2022</b> , 4,	1
75	High-Dimensional Neural Network Potential for Liquid Electrolyte Simulations. <b>2022</b> , 126, 6271-6280	2
74	Benefits of Range-Separated Hybrid and Double-Hybrid Functionals for a Large and Diverse Data Set of Reaction Energies and Barrier Heights. <b>2022</b> , 126, 5492-5505	1
73	Non-Dyson Algebraic Diagrammatic Construction Theory for Charged Excitations in Solids.	1
72	DFT-1/2 and shell DFT-1/2 methods: electronic structure calculation for semiconductors at LDA complexity. <b>2022</b> , 34, 403001	2
71	Boron adatom adsorption on graphene: A case study in computational chemistry methods for surface interactions. 10,	1
70	Correct and Accurate Polymorphic Energy Ordering of Transition-Metal Monoxides Obtained from Semilocal and Onsite-Hybrid Exchange-Correlation Approximations.	О
69	Electronic correlation in nearly free electron metals with beyond-DFT methods. 2022, 8,	О
68	Self-Consistent Implementation of KohnBham Adiabatic Connection Models with Improved Treatment of the Strong-Interaction Limit.	О
67	Understanding speciation and solvation of glyphosate from first principles simulations. <b>2022</b> , 365, 120154	O
66	Redesigning density functional theory with machine learning. 2023, 531-558	О
65	Density-functional theory. <b>2023</b> , 27-65	Ο

64	Computational aspects to design iridium complexes as emitters for OLEDs. 2022, 7, 1172-1206	0
63	DFT Exchange: Sharing Perspectives on the Workhorse of Quantum Chemistry and Materials Science.	9
62	The DFT Approach to predict 13C NMR chemical shifts of hydrocarbon species adsorbed on Zn-modified zeolites. <b>2022</b> , 24, 22241-22249	0
61	Insights into the high-pressure behavior of solid bromine from hybrid density functional theory calculations. <b>2022</b> , 106,	0
60	Thermodynamics and dielectric response of BaTiO3 by data-driven modeling. 2022, 8,	0
59	The performance of exchangeflorrelation functionals in describing electron density parameters of saddle point structures along chemical reactions. <b>2022</b> , 43, 1830-1838	O
58	Evolving symbolic density functionals. <b>2022</b> , 8,	1
57	Importance of imposing gauge invariance in time-dependent density functional theory calculations with meta-generalized gradient approximations. <b>2022</b> , 157, 111102	O
56	Scaled Functionals for the KohnBham correlation energy with scaling functions from the homogeneous electron gas. <b>2022</b> , 157, 114105	1
55	Cheap Turns Superior: A Linear Regression-Based Correction Method to Reaction Energy from the DFT.	O
54	Reduced-Scaling Double Hybrid Density Functional Theory with Rapid Basis Set Convergence through Localized Pair Natural Orbital F12. 9332-9338	1
53	Explicitly Correlated Double-Hybrid DFT: A Comprehensive Analysis of the Basis Set Convergence on the GMTKN55 Database.	3
52	Best-Practice DFT Protocols for Basic Molecular Computational Chemistry**.	2
51	Best-Practice DFT Protocols for Basic Molecular Computational Chemistry**.	10
50	Challenges, Opportunities, and Prospects in Metal Halide Perovskites from Theoretical and Machine Learning Perspectives. 2202279	2
49	How good are recent density functionals for ground and excited states of one-electron systems?.	0
48	Sensitivity of coupled cluster electronic properties on the reference determinant: Can KohnBham orbitals be more beneficial than HartreeBock orbitals?.	1
47	Comparison of Density-Matrix Corrections to Density Functional Theory.	О

46	Non-empirical double-hybrid density functionals as reliable tools for electronic structure calculations. <b>2022</b> , 4, 043001	1
45	Many recent density functionals are numerically ill-behaved.	1
44	PtOxCly(OH)z(H2O)n Complexes under Oxidative and Reductive Conditions Impact of the Level of Theory on Thermodynamic Stabilities.	О
43	First-principles electronic structure investigation of HgBa2CanflCunO2n+2+x with the SCAN density functional. <b>2022</b> , 12, 105308	O
42	The fourth-order expansion of the exchange hole and neural networks to construct exchangeBorrelation functionals. <b>2022</b> , 157, 171103	O
41	Exact constraints and appropriate norms in machine-learned exchange-correlation functionals. <b>2022</b> , 157, 174106	2
40	Accurate path-integral molecular dynamics calculation of aluminum with improved empirical ionic potentials. <b>2022</b> , 106,	О
39	Efficient Method for the Computation of Frozen-Core Nuclear Gradients within the Random Phase Approximation.	O
38	A comprehensive benchmark investigation of quantum chemical methods for carbocations.	О
37	Does GLPT2 offer any actual benefit over conventional HF-MP2 in the context of double-hybrid density functionals?. <b>2022</b> ,	1
36	Multiscale Computational Approaches toward the Understanding of Materials. 2200628	1
35	Spin-State Splittings in 3d Transition-Metal Complexes Revisited: Benchmarking Approximate Methods for Adiabatic Spin-State Energy Differences in Fe(II) Complexes. <b>2022</b> , 18, 7442-7456	1
34	Testing of Exchange-Correlation Functionals of DFT for a Reliable Description of the Electron Density Distribution in Organic Molecules. <b>2022</b> , 23, 14719	1
33	SBH17: Benchmark Database of Barrier Heights for Dissociative Chemisorption on Transition Metal Surfaces.	1
32	Modeling the electronic structure of organic materials: a solid-state physicist⊠ perspective. <b>2023</b> , 6, 012001	О
31	Geometries and vibrational frequencies with Kohn-Sham methods using \$sigma\$-functionals for the correlation energy.	O
30	Double Hybrid Density Functionals for the Electronic Excitation Energies of Linear Cyanines.	О
29	Behavior of HF and (HF) 2 inside a fullerene cage: An in silico study using different density functionals.	O

28	Interexcited State Photophysics I: Benchmarking Density Functionals for Computing Nonadiabatic Couplings and Internal Conversion Rate Constants.	О
27	Mean Value Ensemble Hubbard-U Correction for Spin-Crossover Molecules. 12049-12054	О
26	A transferable recommender approach for selecting the best density functional approximations in chemical discovery.	1
25	Role of Single-atom Rh-dopants in the Adsorption Properties of OH and CO on Stepped Ag(211).	O
24	Full Implementation, Optimization, and Evaluation of a Range-Separated Local Hybrid Functional with Wide Accuracy for Ground and Excited States.	0
23	Emergence of Wigner oscillations in a model of real time cooling process: a time-dependent density-functional theory approach. <b>2023</b> , 35, 115602	0
22	Data-driven many-body potentials from density functional theory for aqueous phase chemistry. <b>2023</b> , 4, 011301	0
21	A machine learning route between band mapping and band structure.	o
20	Symmetry Breaking with the SCAN Density Functional Describes Strong Correlation in the Singlet Carbon Dimer. <b>2023</b> , 127, 384-389	2
19	Inversion Theory Leveling as a New Methodological Approach to Antioxidant Thermodynamics: A Case Study on Phenol. <b>2023</b> , 12, 282	o
18	Emerging Trends of Computational Chemistry and Molecular Modeling in Froth Flotation: A Review.	O
17	Spin-state gaps and self-interaction-corrected density functional approximations: Octahedral Fe(II) complexes as case study. <b>2023</b> , 158, 054305	o
16	Understanding the adsorption behavior of oxygen on the 3CBiC(1 1 0) surface: A first-principles study. <b>2023</b> , 106, 3676-3687	0
15	Recent progress of theoretical research on inorganic solid state electrolytes for Li metal batteries. <b>2023</b> , 561, 232720	1
14	Ab Initio Static Exchangetorrelation Kernel across Jacoba Ladder without Functional Derivatives. <b>2023</b> , 19, 1286-1299	2
13	Molecular Understanding and Practical In Silico Catalyst Design in Computational Organocatalysis and Phase Transfer Catalysis Thallenges and Opportunities. <b>2023</b> , 28, 1715	0
12	Insights into the deviation from piecewise linearity in transition metal complexes from supervised machine learning models. <b>2023</b> , 25, 8103-8116	0
11	A new freely-downloadable hands-on density-functional theory workbook using a freely-downloadable version of deMon2k. <b>2023</b> ,	О

#### CITATION REPORT

10	Exhaust Gases as Fluxing Agents for Palladium: Formation Enthalpies and Vapor Pressures of PdO, PdO2, Pd(CO)n (n = 1B), Pd(NO)n (n = 1,2), Pd(OH)n (n = 1,2), HOPdNO, and 21 Other Species under Automotive Catalyst Aging Conditions. <b>2023</b> , 127, 4917-4933	О
9	Electronic density response of warm dense matter. <b>2023</b> , 30, 032705	2
8	Four-Component Relativistic Calculations of NMR Shielding Constants of the Transition Metal ComplexesPart 3: Fe, Co, Ni, Pd, and Pt Glycinates. <b>2023</b> , 9, 83	О
7	Investigating the Thermodynamics and Kinetics of Catechin Pyrolysis for Environmentally Friendly Binders. <b>2023</b> , 8, 12693-12701	O
6	Seven useful questions in density functional theory. <b>2023</b> , 113,	O
5	Performance of Common Density Functionals for Excited States of Tetraphenyldibenzoperiflanthene. <b>2023</b> , 127, 3265-3273	O
4	Comparison of the Performance of Density Functional Methods for the Description of Spin States and Binding Energies of Porphyrins. <b>2023</b> , 28, 3487	O
3	Enabling Molecular-Level Computational Description of Redox and Proton-Coupled Electron Transfer Reactions of Samarium Diiodide.	O
2	A semilocal machine-learning correction to density functional approximations. 2023, 158,	О
1	Performance of Functionals and Basis Sets in Calculating Redox Potentials of Nitrile Alkenes and Aromatic Molecules using Density Functional Theory. <b>2023</b> , 8,	O