Density functional theory: Its origins, rise to prominent

Reviews of Modern Physics 87, 897-923

DOI: 10.1103/revmodphys.87.897

Citation Report

#	Article	IF	CITATIONS
2	Phonon effects on x-ray absorption and nuclear magnetic resonance spectroscopies. Physical Review B, $2015, 92, .$	3.2	31
3	Comparing the Models of Steepest Entropy Ascent Quantum Thermodynamics, Master Equation and the Difference Equation for a Simple Quantum System Interacting with Reservoirs. Entropy, 2016, 18, 176.	2.2	7
4	Assessing the accuracy of improved forceâ€matched water models derived from <i>Ab initio</i> molecular dynamics simulations. Journal of Computational Chemistry, 2016, 37, 1828-1838.	3.3	11
5	The virtual atomic and molecular data centre (VAMDC) consortium. Journal of Physics B: Atomic, Molecular and Optical Physics, 2016, 49, 074003.	1.5	120
6	Ab initioderivation of model energy density functionals. Journal of Physics G: Nuclear and Particle Physics, 2016, 43, 04LT01.	3.6	30
7	Hartree potential dependent exchange functional. Journal of Chemical Physics, 2016, 145, 084110.	3.0	15
8	Increasing the applicability of density functional theory. V. X-ray absorption spectra with ionization potential corrected exchange and correlation potentials. Journal of Chemical Physics, 2016, 145, 034108.	3.0	22
9	Perspective: Role of structure prediction in materials discovery and design. APL Materials, 2016, 4, 053210.	5.1	114
10	Inapplicability of exact constraints and a minimal two-parameter generalization to the DFT+ <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mi>U</mml:mi></mml:math> based correction of self-interaction error. Physical Review B, 2016, 94, .	3.2	10
11	Structural properties of Co2TiSi films on GaAs(001). Journal of Applied Physics, 2016, 120, .	2.5	1
12	Research Update: The materials genome initiative: Data sharing and the impact of collaborative $\langle i \rangle$ ab initio $\langle i \rangle$ databases. APL Materials, 2016, 4, .	5.1	115
13	Nucleon localization and fragment formation in nuclear fission. Physical Review C, 2016, 94, .	2.9	44
14	The QTP family of consistent functionals and potentials in Kohn-Sham density functional theory. Journal of Chemical Physics, 2016, 145, 034107.	3.0	68
15	Theoretical simulations on the antioxidant mechanism of naturally occurring flavonoid: A DFT approach. AIP Conference Proceedings, 2016, , .	0.4	3
16	Rungs 1 to 4 of DFT Jacob's ladder: Extensive test on the lattice constant, bulk modulus, and cohesive energy of solids. Journal of Chemical Physics, 2016, 144, 204120.	3.0	191
17	Calculation of 2D electronic band structure using matrix mechanics. American Journal of Physics, 2016, 84, 924-935.	0.7	13
18	Empirical relation between Pauling electronegativity and self-energy cutoffs in local-density approximation-1/2 quasi-particle approach applied to the calculation of band gaps of binary compound semiconductors. MRS Communications, 2016, 6, 99-103.	1.8	6
19	Influence of the exchange and correlation functional on the structure of amorphous InSb and In3SbTe2 compounds. Journal of Chemical Physics, 2016, 144, 204508.	3.0	8

#	Article	IF	Citations
20	Diffraction at GaAs/Fe3Si core/shell nanowires: The formation of nanofacets. AIP Advances, 2016, 6, .	1.3	2
21	Collective excitations and viscosity in liquid Bi. Journal of Chemical Physics, 2016, 145, 184502.	3.0	16
22	Locality of correlation in density functional theory. Journal of Chemical Physics, 2016, 145, 054112.	3.0	35
23	Nuclear Structure Models Based on Relativistic Energy Density Functionals. Springer Proceedings in Physics, 2016, , 113-165.	0.2	0
24	Theoretical study on gas decomposition mechanism of SF6 by quantum chemical calculation. Computational and Theoretical Chemistry, 2016, 1088, 24-31.	2.5	21
25	Electronic structure and optical properties of CsI, CsI(Ag), and CsI(Tl). Journal of the Korean Physical Society, 2016, 68, 1069-1074.	0.7	14
26	New developments in classical density functional theory. Journal of Physics Condensed Matter, 2016, 28, 240401.	1.8	71
27	Dense ionic fluids confined in planar capacitors: in- and out-of-plane structure from classical density functional theory. Journal of Physics Condensed Matter, 2016, 28, 244007.	1.8	15
28	Dyes and Pigments. Springer Briefs in Molecular Science, 2016, , .	0.1	79
29	Dyes and Pigments: Their Structure and Properties. Springer Briefs in Molecular Science, 2016, , 13-29.	0.1	80
30	A first-principles based study of ns ² containing ternary iodides and their possibility of scintillation. Journal Physics D: Applied Physics, 2016, 49, 395103.	2.8	9
31	Structural, Electronic, and Optical Properties of Bulk Boric Acid <i>2A</i> and <i>3T</i> Polymorphs: Experiment and Density Functional Theory Calculations. Crystal Growth and Design, 2016, 16, 6631-6640.	3.0	13
32	Integrated Strategy toward Self-Powering and Selectivity Tuning of Semiconductor Gas Sensors. ACS Sensors, 2016, 1, 1256-1264.	7.8	28
33	Hexagonal structure of phase III of solid hydrogen. Physical Review B, 2016, 94, .	3.2	44
34	Applications of large-scale density functional theory in biology. Journal of Physics Condensed Matter, 2016, 28, 393001.	1.8	105
35	Multi-step reaction mechanism for F atom interactions with organosilicate glass and SiO _{<i>x</i>} films. Journal Physics D: Applied Physics, 2016, 49, 345203.	2.8	21
36	Kineticâ€energyâ€density dependent semilocal exchangeâ€correlation functionals. International Journal of Quantum Chemistry, 2016, 116, 1641-1694.	2.0	78
37	Stability and accuracy control of k \hat{A} p parameters. Semiconductor Science and Technology, 2016, 31, 105002.	2.0	11

#	ARTICLE	IF	CITATIONS
38	Stability and geometry of silica nano-ribbons (SNRs): a first-principles study. Physical Chemistry Chemical Physics, 2016, 18, 21825-21832.	2.8	3
39	One- and many-electron self-interaction error in local and global hybrid functionals. Physical Review B, 2016, 93, .	3.2	62
40	Bond-order potential for magnetic body-centered-cubic iron and its transferability. Physical Review B, 2016, 93, .	3.2	14
41	Quantum ring-polymer contraction method: Including nuclear quantum effects at no additional computational cost in comparison to <i>ab initio</i> molecular dynamics. Physical Review E, 2016, 93, 043305.	2.1	31
42	Dynamical screening in correlated electron systemsâ€"from lattice models to realistic materials. Journal of Physics Condensed Matter, 2016, 28, 383001.	1.8	50
43	Electron density distribution and electronic structure as tools to study the origin of ferroic states in ferroelectric and magnetic materials. Ferroelectrics, 2016, 500, 26-36. Crystallization processes in the phase change material <mml:math< td=""><td>0.6</td><td>2</td></mml:math<>	0.6	2
44	xmlns:mml="http://www.w3.org/1998/Math/MathML"> <mml:mrow><mml:msub><mml:mi mathvariant="bold">Ge</mml:mi><mml:mn>2</mml:mn></mml:msub><mml:msub><mml:mi mathvariant="bold">Sb</mml:mi><mml:mn>2</mml:mn></mml:msub><mml:msub><mml:mi mathvariant="bold">Te</mml:mi><mml:mn>5</mml:mn></mml:msub></mml:mrow> :	3.2	57
45	Unbiased density functional/molecular dynamics simulations. Physical Review B, 2016, 94, . First-Principles Monte Carlo Simulations of Reaction Equilibria in Compressed Vapors. ACS Central Science, 2016, 2, 409-415.	11.3	16
46	Oxygen vacancy promoted methane partial oxidation over iron oxide oxygen carriers in the chemical looping process. Physical Chemistry Chemical Physics, 2016, 18, 32418-32428.	2.8	88
47	Systematic construction of density functionals based on matrix product state computations. New Journal of Physics, 2016, 18, 083039.	2.9	16
48	Insights into phase transitions and entanglement from density functional theory. New Journal of Physics, 2016, 18, 113035.	2.9	6
49	Insights into the spurious long-range nature of local rs-dependent non-local exchange-correlation kernels. Journal of Chemical Physics, 2016, 145, 054121.	3.0	0
50	Electrons and phonons in amorphous semiconductors. Semiconductor Science and Technology, 2016, 31, 073002.	2.0	31
51	Amp: A modular approach to machine learning in atomistic simulations. Computer Physics Communications, 2016, 207, 310-324.	7.5	281
52	Fluorine-Terminated Diamond Surfaces as Dense Dipole Lattices: The Electrostatic Origin of Polar Hydrophobicity. Journal of the American Chemical Society, 2016, 138, 4018-4028.	13.7	47
53	Reproducibility in density functional theory calculations of solids. Science, 2016, 351, aad3000.	12.6	1,113
54	Spinâ€"Orbit Effects in Closed-Shell Heavy and Superheavy Element Monohydrides and Monofluorides with Coupled-Cluster Theory. Journal of Physical Chemistry A, 2016, 120, 1231-1242.	2.5	22
55	First-principles calculations of thermal, electrical, and thermoelectric transport properties of semiconductors. Semiconductor Science and Technology, 2016, 31, 043001.	2.0	51

#	Article	IF	CITATIONS
56	Nonclassical Plasmonics. Springer Theses, 2017, , 37-80.	0.1	1
57	Density functional theory is straying from the path toward the exact functional. Science, 2017, 355, 49-52.	12.6	711
58	Deciphering chemical order/disorder and material properties at the single-atom level. Nature, 2017, 542, 75-79.	27.8	243
59	Temperature dependence of X-ray absorption and nuclear magnetic resonance spectra: probing quantum vibrations of light elements in oxides. Physical Chemistry Chemical Physics, 2017, 19, 6246-6256.	2.8	16
60	Three-dimensional organic Dirac-line materials due to nonsymmorphic symmetry: A data mining approach. Physical Review B, 2017, 95, .	3.2	29
61	Electronic structure and optical properties of the scintillation material wurtzite ZnS(Ag). Nuclear Science and Techniques/Hewuli, 2017, 28, 1.	3.4	7
62	The screened pseudo-charge repulsive potential in perturbed orbitals for band calculations by DFT+U. Physical Chemistry Chemical Physics, 2017, 19, 8008-8025.	2.8	40
63	Energetics of <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:msub><mml:mi mathvariant="normal">H</mml:mi><mml:mn>2</mml:mn></mml:msub></mml:math> clusters from density functional and coupled cluster theories. Physical Review B, 2017, 95, .	3.2	2
64	Can X-ray constrained Hartree–Fock wavefunctions retrieve electron correlation?. IUCrJ, 2017, 4, 136-146.	2.2	44
65	Stratified construction of neural network based interatomic models for multicomponent materials. Physical Review B, 2017, 95, .	3.2	67
66	Asymmetric hydrogen bonding in formic acid–nitric acid dimer observed by quantum molecular dynamics simulations. Theoretical Chemistry Accounts, 2017, 136, 1.	1.4	2
67	Ion beam modification of two-dimensional materials: Characterization, properties, and applications. Applied Physics Reviews, 2017, 4, 011103.	11.3	168
68	Free energy of the uniform electron gas: Testing analytical models against firstâ€principles results. Contributions To Plasma Physics, 2017, 57, 137-146.	1.1	25
69	Kinetic energy partition method applied to ground state helium-like atoms. Journal of Chemical Physics, 2017, 146, 124120.	3.0	7
70	What Makes a Density Functional Approximation Good? Insights from the Left Fukui Function. Journal of Chemical Theory and Computation, 2017, 13, 2373-2377.	5.3	33
71	Atomicrex—a general purpose tool for the construction of atomic interaction models. Modelling and Simulation in Materials Science and Engineering, 2017, 25, 055003.	2.0	18
72	Towards a metal-semiconductor transition in two dimensions. Chemical Physics Letters, 2017, 679, 127-131.	2.6	4
73	Missing Fe: hydrogenated iron nanoparticles. Monthly Notices of the Royal Astronomical Society: Letters, 2017, 466, L14-L18.	3.3	11

#	ARTICLE	IF	CITATIONS
74	Dispersion-Corrected Spin-Component-Scaled Double-Hybrid Density Functional Theory: Implementation and Performance for Non-covalent Interactions. Journal of Chemical Theory and Computation, 2017, 13, 2650-2666.	5.3	8
75	Route towards Dirac and Weyl antiferromagnetic spintronics. Physica Status Solidi - Rapid Research Letters, 2017, 11, 1700044.	2.4	51
76	The atomic simulation environmentâ€"a Python library for working with atoms. Journal of Physics Condensed Matter, 2017, 29, 273002.	1.8	1,933
77	Opinion: Quantum solutions for a sustainable energy future. Nature Reviews Chemistry, 2017, $1, .$	30.2	18
78	Single-particle excitation of core states in epitaxial silicene. Physical Review B, 2017, 95, .	3.2	13
79	Kinetic energy density for orbitalâ€free density functional calculations by axiomatic approach. International Journal of Quantum Chemistry, 2017, 117, e25373.	2.0	9
80	Dirac's dream: Understanding metal sorption by geomedia using density functional theory. Chemical Geology, 2017, 464, 4-13.	3.3	16
81	<i>Ab initio</i> quantum Monte Carlo simulation of the warm dense electron gas. Physics of Plasmas, 2017, 24, .	1.9	59
82	Conformational Populations of \hat{I}^2 -($1\hat{a}^{\dagger}$ '4) <i>O</i> -Glycosidic Linkages Using Redundant NMR <i>J</i> -Couplings and Circular Statistics. Journal of Physical Chemistry B, 2017, 121, 3042-3058.	2.6	39
83	SPARC: Accurate and efficient finite-difference formulation and parallel implementation of Density Functional Theory: Extended systems. Computer Physics Communications, 2017, 216, 109-125.	7.5	109
84	First-principles study of the dynamic Jahn-Teller distortion of the neutral vacancy in diamond. Physical Review B, 2017 , 95 , .	3.2	23
85	Emerging New Pseudobinary and Ternary Halides as Scintillators for Radiation Detection. IEEE Transactions on Nuclear Science, 2017, 64, 1817-1824.	2.0	9
86	Classical Density Functional Theory for Molecular Systems. Molecular Modeling and Simulation, 2017, , 65-99.	0.2	9
87	Multi-fidelity machine learning models for accurate bandgap predictions of solids. Computational Materials Science, 2017, 129, 156-163.	3.0	235
88	Theoretical Investigation of Electronic Properties of Undoped and Ag-Doped (CdTe)16×N Multi-cage Nanochains. Journal of Cluster Science, 2017, 28, 1393-1405.	3.3	2
89	Thermal quenching of Eu 2+ emission in Ca- and Sr-Ga 2 S 4 in relation with VRBE schemes. Journal of Luminescence, 2017, 184, 256-261.	3.1	11
90	Computational design of two-dimensional nanomaterials for charge modulated CO2/H2 capture and/or storage. Energy Storage Materials, 2017, 8, 169-183.	18.0	25
91	<i>AbÂinitio</i> Exchange-Correlation Free Energy of the Uniform Electron Gas at Warm Dense Matter Conditions. Physical Review Letters, 2017, 119, 135001.	7.8	139

#	ARTICLE	IF	CITATIONS
92	Stability, local structure and electronic properties of borane radicals on the Si(1 0 0) 2 \tilde{A} — 1:H surface: A first-principles study. Computational Materials Science, 2017, 140, 253-260.	3.0	3
93	Electronic correlations in vanadium revealed by electron-positron annihilation measurements. Physical Review B, 2017, 95, .	3.2	8
95	Picoscale materials engineering. Nature Reviews Materials, 2017, 2, .	48.7	42
96	First-principles calculations of Co 7 W 6 doped with Re: Site occupancy and electronic properties. Computational Condensed Matter, 2017, 13, 36-40.	2.1	4
97	Structure of electric double layers in capacitive systems and to what extent (classical) density functional theory describes it. Journal of Physics Condensed Matter, 2017, 29, 423002.	1.8	39
98	Efficient Implicit Solvation Method for Full Potential DFT. Journal of Chemical Theory and Computation, 2017, 13, 5582-5603. Structural and electronic properties of <mml:math< td=""><td>5.3</td><td>30</td></mml:math<>	5.3	30
99	xmlns:mml="http://www.w3.org/1998/Math/MathML"> <mml:mi>α</mml:mi> -(BEDT-TTF) <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mrow><mml:msub><mml:mrow></mml:mrow><mml:mn>2</mml:mn></mml:msub><mml:mi mathvariant="normal">I</mml:mi><mml:mn>3</mml:mn></mml:mrow></mml:math> <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mi>β</mml:mi></mml:math>		

#	ARTICLE Point defects in the <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mrow><mml:mn>1</mml:mn><mml:msup><mml< th=""><th>IF ·mi>Te/mn</th><th>CITATIONS</th></mml<></mml:msup></mml:mrow></mml:math>	IF ·mi>Te/mn	CITATIONS
111	and <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mrow><mml:mn>2</mml:mn><mml:mi>Hphases of single-layer <mml:math< td=""><td>mi></td><td>mrow></td></mml:math<></mml:mi></mml:mrow></mml:math>	mi>	mrow>
112	xmlns:mml="http://www.w3.org/1998/Math/MathML"> <mml:msub><mml:mi>MoS</mml:mi><mml:mn>2Changing the gap type of solid state boric acid by heating: a dispersion-corrected density functional study of l±-, l²-, and l³-metaboric acid polymorphs. New Journal of Chemistry, 2017, 41, 15533-15544.</mml:mn></mml:msub>	nl:mn>2.8	ml:msub>4
113	Covalent Bonding in the Hydrogen Molecule. Journal of Physical Chemistry A, 2017, 121, 9330-9345.	2.5	15
114	Crystallization of supercooled liquid antimony: A density functional study. Physical Review B, 2017, 96,	3.2	20
115	Understanding the behavior of caffeine on a boron-doped diamond surface: voltammetric, DFT, QTAIM and ELF studies. New Journal of Chemistry, 2017, 41, 7766-7774.	2.8	18
116	Density functional study of structure and dynamics in liquid antimony and Sb <i>n</i> clusters. Journal of Chemical Physics, 2017, 146, 194502.	3.0	15
117	Reactive pathways of hydrogen and carbon removal from organosilicate glass low- \hat{l}^2 films by F atoms. European Physical Journal D, 2017, 71, 1.	1.3	7
118	Full-valence density matrix renormalisation group calculations on meta-benzyne based on unrestricted natural orbitals. Revisit of seamless continuation from broken-symmetry to symmetry-adapted models for diradicals. Molecular Physics, 2017, 115, 2267-2284.	1.7	14
119	Nanoscale capacitance: A quantum tight-binding model. Physics Letters, Section A: General, Atomic and Solid State Physics, 2017, 381, 44-47.	2.1	0
120	Computing partial traces and reduced density matrices. International Journal of Modern Physics C, 2017, 28, 1750005.	1.7	16
121	Titania–silica mixed oxides investigated with density functional theory and molecular dynamics simulations. Physica Status Solidi (B): Basic Research, 2017, 254, 1600510.	1.5	5
122	SPARC: Accurate and efficient finite-difference formulation and parallel implementation of Density Functional Theory: Isolated clusters. Computer Physics Communications, 2017, 212, 189-204.	7. 5	71
123	New insights about the hydrogen bonds formed between acetylene and hydrogen fluoride: \ddot{l} € \hat{a} H, C \hat{a} H and F \hat{a} H. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2017, 173, 160-169.	3.9	10
124	Variational quantum Monte Carlo results for N _{2} , N _{2} ^{–} utili s ing the four-dimensional density of Bright Wilson. Physics and Chemistry of Liquids, 2017, 55, 281-290.	1.2	1
125	Complex structure of optical transitions from the core d-levels of InAs and InSb crystals. Semiconductors, 2017, 51, 1034-1040.	0.5	1
126	Dielectric permeability tensor and linear waves in spin-1/2 quantum kinetics with non-trivial equilibrium spin-distribution functions. Physics of Plasmas, 2017, 24, 112108.	1.9	9
127	Phase stability and elastic properties of <i>β</i> Ti–Nb– <i>X</i> (<i>X</i> = Zr, Sn) alloys: an <i>ab initio</i> density functional study. Modelling and Simulation in Materials Science and Engineering, 2017, 25, 085013.	2.0	10
128	When combined X-ray and polarized neutron diffraction data challenge high-level calculations: spin-resolved electron density of an organic radical. Acta Crystallographica Section B: Structural Science, Crystal Engineering and Materials, 2017, 73, 544-549.	1.1	13

#	ARTICLE	IF	CITATIONS
129	Prediction and characterization of an Mg-Al intermetallic compound with potentially improved ductility via orbital-free and Kohn-Sham density functional theory. Modelling and Simulation in Materials Science and Engineering, 2017, 25, 075002.	2.0	11
130	Quantum Monte Carlo Study of Buckled GaAs Monolayer. Macromolecular Symposia, 2017, 376, 1600206.	0.7	2
131	Class of diatomic ferroelectrics with multifunctional properties: IV-VI compounds in the distorted NiAs-type structure. Physical Review B, 2017, 96, .	3.2	4
132	Neutron total cross section calculation within the framework of quasi-harmonic approximation. New Journal of Physics, 2017, 19, 103027.	2.9	7
133	First-Principles View on Photoelectrochemistry: Water-Splitting as Case Study. Inorganics, 2017, 5, 37.	2.7	22
134	Organic materials database: An open-access online database for data mining. PLoS ONE, 2017, 12, e0171501.	2.5	65
135	Electronic Effect of V, Ti, and Sc Impurities on the Hyperfine Interactions of Fe Atoms in \hat{l}_{\pm} -Fe: A First Principles Study. Materials Research, 2017, 20, 523-531.	1.3	3
136	Post-B3LYP Functionals Do Not Improve the Description of Magnetic Coupling in Cu(II) Dinuclear Complexes. Journal of Physical Chemistry A, 2018, 122, 3423-3432.	2.5	12
137	Single-layer 1 <i>T</i> ′-MoS ₂ under electron irradiation from <i>ab initio</i> molecular dynamics. 2D Materials, 2018, 5, 025022.	4.4	13
138	Bonding in phase change materials: concepts and misconceptions. Journal of Physics Condensed Matter, 2018, 30, 153001.	1.8	16
139	Functional renormalization group and Kohn–Sham scheme in density functional theory. Physics Letters, Section B: Nuclear, Elementary Particle and High-Energy Physics, 2018, 779, 436-440.	4.1	23
140	Tetrahedral hydrocarbon nanoparticles in space: X-ray spectra. Monthly Notices of the Royal Astronomical Society, 2018, 476, 5358-5364.	4.4	5
141	Structural, electronic and optical properties of LiNbO ₃ using GGA-PBE and TB-mBJ functionals: A DFT study. International Journal of Modern Physics B, 2018, 32, 1850168.	2.0	26
142	Benchmarks and Reliable DFT Results for Spin Gaps of Small Ligand Fe(II) Complexes. Journal of Chemical Theory and Computation, 2018, 14, 2304-2311.	5.3	71
143	In silico methods in forensic science: Quantum chemistry and multivariate analysis applied to infrared spectra of new amphetamine- and cathinone-derived psychoactive substances. Forensic Chemistry, 2018, 9, 21-34.	2.8	9
144	Stochastic sampling of quadrature grids for the evaluation of vibrational expectation values. Physical Review B, 2018, 97, .	3.2	1
145	A new look at acid catalyzed deacetylation of carbohydrates: A regioselective synthesis and reactivity of 2-O-acetyl aryl glycopyranosides. Carbohydrate Research, 2018, 458-459, 60-66.	2.3	7
146	Verdazyl Radical Building Blocks: Synthesis, Structure, and Sonogashira Cross oupling Reactions. European Journal of Organic Chemistry, 2018, 2018, 4802-4811.	2.4	23

#	Article	IF	CITATIONS
147	Tutorial: Junction spectroscopy techniques and deep-level defects in semiconductors. Journal of Applied Physics, $2018,123,123$	2.5	82
148	Semiclassical dynamics of spin density waves. Physical Review B, 2018, 97, .	3.2	27
149	The uniform electron gas at warm dense matter conditions. Physics Reports, 2018, 744, 1-86.	25.6	177
150	Electronic effects and fundamental physics studied in molecular interfaces. Chemical Communications, 2018, 54, 5508-5517.	4.1	5
151	First-principles calculations of the stibnite at the level of modified Becke–Johnson exchange potential. Chinese Journal of Physics, 2018, 56, 1331-1344.	3.9	10
152	Charge transfer excitations from exact and approximate ensemble Kohn-Sham theory. Journal of Chemical Physics, 2018, 148, 174101.	3.0	29
153	Industrial application of molecular computations on the dimerization of methylene diphenyl disocyanate. Reaction Kinetics, Mechanisms and Catalysis, 2018, 124, 1-14.	1.7	4
154	xmlns:mml="http://www.w3.org/1998/Math/MathML"> <mml:msub><mml:mi mathvariant="normal">N</mml:mi><mml:mn>2</mml:mn></mml:msub> by <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:msup><mml:mrow><mml:mi mathvariant="normal">H</mml:mi>></mml:mrow></mml:msup></mml:math>	2.5	11
155	Impact at keV energies within time-dependent density-functional theory. Physical Review A, 2018, 97, How Accurate Is Density Functional Theory at Predicting Dipole Moments? An Assessment Using a New Database of 200 Benchmark Values. Journal of Chemical Theory and Computation, 2018, 14, 1969-1981.	5.3	180
156	Experimental and computational approaches to the analysis of the molecular structure of (E)-3-(3-(4-nitrophenyl)triaz-1-en-1-yl)-1H-pyrazole-4-carbonitrile. Journal of Molecular Structure, 2018, 1155, 239-248.	3.6	5
157	Ab-initio study of electronic and elastic properties of Mg(BH4)(NH2) complex hydride. International Journal of Hydrogen Energy, 2018, 43, 1587-1595.	7.1	3
158	Structure-dependent luminescence of tetra-(4-pyridylphenyl)ethylene: a first-principles study. Physical Chemistry Chemical Physics, 2018, 20, 41-45.	2.8	4
159	Solving many-body Schrödinger equations with kinetic energy partition method. Annals of Physics, 2018, 388, 54-68.	2.8	2
160	Scaling behavior of the Compton profile of alkali metals. Physica A: Statistical Mechanics and Its Applications, 2018, 489, 18-27.	2.6	6
161	Building bridges: matching density functional theory with experiment. Contemporary Physics, 2018, 59, 377-390.	1.8	0
162	Electronic Structure and Magnetic Properties of Strongly Correlated Transition Metal Compounds. Physics of Metals and Metallography, 2018, 119, 1254-1258.	1.0	5
164	â€~Diet GMTKN55' offers accelerated benchmarking through a representative subset approach. Physical Chemistry Chemical Physics, 2018, 20, 27735-27739.	2.8	26
165	Interplay between test sets and statistical procedures in ranking DFT methods: The case of electron density studies. Mendeleev Communications, 2018, 28, 225-235.	1.6	36

#	Article	IF	CITATIONS
167	Independent amplitude approximations in coupled cluster valence bond theory: Incorporation of 3-electron-pair correlation and application to spin frustration in the low-lying excited states of a ferredoxin-type tetrametallic iron-sulfur cluster. Journal of Chemical Physics, 2018, 149, 144103.	3.0	7
168	Multilevel Approach for Direct VSCF/VCI MULTIMODE Calculations with Applications to Large "Zundel―Cations. Journal of Chemical Theory and Computation, 2018, 14, 6405-6416.	5.3	11
169	Visualizing atomic sizes and molecular shapes with the classical turning surface of the Kohn–Sham potential. Proceedings of the National Academy of Sciences of the United States of America, 2018, 115, E11578-E11585.	7.1	27
170	Melting a Hubbard dimer: benchmarks of †ALDA†for quantum thermodynamics. European Physical Journal B, 2018, 91, 1.	1.5	7
171	Ionicity of bonding in elemental solids. Journal of Physics Communications, 2018, 2, 115009.	1.2	3
172	Role of spin in the calculation of Hubbard <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mi>U</mml:mi></mml:math> and Hund's <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mi>J</mml:mi></mml:math> parameters from first principles. Physical Review B. 2018. 98	3.2	45
173	Communication: Relating the pure and ensemble density matrix functional. Journal of Chemical Physics, 2018, 149, 231102.	3.0	37
174	Efficient O(<mml:math) (xmlns:mml="http://www.w3.org/1 divide-conquer method with localized single-particle natural orbitals. Physical Review B, 2018, 98, .</td><td>998/Math/
3.2</td><td>MathML" 0.784314="" 1="" 10="" 467="" 50="" etqq1="" overlock="" rgbt="" td="" tf="" tj=""> < 2</mml:math)>		
175	Phase transition systematics in <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:msub><mml:mi>BiVO</mml:mi><mml:mn>4<td>ന്ങ2<td>:masub></td></td></mml:mn></mml:msub></mml:math>	ന് ങ2 <td>:masub></td>	:masub>
176	Perspectives on the Theory of Defects. Frontiers in Materials, 2018, 5, .	2.4	21
176 177	Perspectives on the Theory of Defects. Frontiers in Materials, 2018, 5, . First principles calculation of spin-related quantities for point defect qubit research. Npj Computational Materials, 2018, 4, .	2.4	21 56
	First principles calculation of spin-related quantities for point defect qubit research. Npj		
177	First principles calculation of spin-related quantities for point defect qubit research. Npj Computational Materials, 2018, 4, . Improving the rectifying performance of the pyrene-benzene system by optimizing its hydrocarbon	8.7	56
177 178	First principles calculation of spin-related quantities for point defect qubit research. Npj Computational Materials, 2018, 4, . Improving the rectifying performance of the pyrene-benzene system by optimizing its hydrocarbon bridge: A first-principles investigation. AIP Advances, 2018, 8, 115128. Density functional electric response properties of molecules in Cartesian grid. International Journal	1.3	56 0
177 178 179	First principles calculation of spin-related quantities for point defect qubit research. Npj Computational Materials, 2018, 4, . Improving the rectifying performance of the pyrene-benzene system by optimizing its hydrocarbon bridge: A first-principles investigation. AIP Advances, 2018, 8, 115128. Density functional electric response properties of molecules in Cartesian grid. International Journal of Quantum Chemistry, 2018, 118, e25708.	1.3	5607
177 178 179	First principles calculation of spin-related quantities for point defect qubit research. Npj Computational Materials, 2018, 4, . Improving the rectifying performance of the pyrene-benzene system by optimizing its hydrocarbon bridge: A first-principles investigation. AIP Advances, 2018, 8, 115128. Density functional electric response properties of molecules in Cartesian grid. International Journal of Quantum Chemistry, 2018, 118, e25708. Density Functional Theory Calculations Applied to Nuclear Fuels. , 2018, , 1-20. Effect of Substrate Chemistry on Prenucleation. Metallurgical and Materials Transactions A: Physical	8.7 1.3 2.0	56071
177 178 179 180	First principles calculation of spin-related quantities for point defect qubit research. Npj Computational Materials, 2018, 4, . Improving the rectifying performance of the pyrene-benzene system by optimizing its hydrocarbon bridge: A first-principles investigation. AIP Advances, 2018, 8, 115128. Density functional electric response properties of molecules in Cartesian grid. International Journal of Quantum Chemistry, 2018, 118, e25708. Density Functional Theory Calculations Applied to Nuclear Fuels., 2018, , 1-20. Effect of Substrate Chemistry on Prenucleation. Metallurgical and Materials Transactions A: Physical Metallurgy and Materials Science, 2018, 49, 6231-6242. Tuned Range-Separated Density Functional Theory and Dyson Orbital Formalism for Photoelectron	8.7 1.3 2.0	56 0 7 1 42

#	Article	IF	CITATIONS
187	Berry Phases and Curvatures. , 0, , 75-140.		1
188	Electric Polarization. , 0, , 141-200.		1
189	Topological Insulators and Semimetals. , 0, , 201-275.		0
190	Orbital Magnetization and Axion Coupling. , 0, , 276-315.		O
197	Delocalization Errors in Density Functional Theory Are Essentially Quadratic in Fractional Occupation Number. Journal of Physical Chemistry Letters, 2018, 9, 6280-6288.	4.6	71
198	Parity-breaking in single-element phases: ferroelectric-like elemental polar metals. Journal of Physics Condensed Matter, 2018, 30, 415504.	1.8	5
199	Accuracy of the Heyd-Scuseria-Ernzerhof hybrid functional to describe many-electron interactions and charge localization in semiconductors. Physical Review B, 2018, 98, .	3.2	13
200	Recent Progress in First-Principles Methods for Computing the Electronic Structure of Correlated Materials. Computation, 2018, 6, 26.	2.0	17
201	Theoretical studies of electronic transport in monolayer and bilayer phosphorene: A critical overview. Physical Review B, 2018, 98, .	3.2	78
202	Vibrational Modes and Phonon and Thermodynamic Properties of the Metaboric Acid Polymorphs $\hat{l}\pm$, \hat{l}^2 , and \hat{l}^3 -(BOH) < sub > 3 < / sub > 0 < sub > 3 < / sub > 0 < sub > 3 < / sub > 0 < sub > 122, 7628-7645.	2.5	4
204	Density Functional Theory for Magnetism and Magnetic Anisotropy. , 2018, , 1-23.		0
206	A review of molecular simulation applied in vapor-liquid equilibria (VLE) estimation of thermodynamic cycles. Journal of Molecular Liquids, 2018, 264, 652-674.	4.9	17
207	Machine Learning and Energy Minimization Approaches for Crystal Structure Predictions: A Review and New Horizons. Chemistry of Materials, 2018, 30, 3601-3612.	6.7	136
208	Optical Transitions in ZnSe and CdTe Crystals with Involvement of the Cation d Bands. Semiconductors, 2018, 52, 287-293.	0.5	0
209	Spectroscopic Studies on the Metalâ€"Insulator Transition Mechanism in Correlated Materials. Advanced Materials, 2018, 30, e1704777.	21.0	18
210	Radical scavenging behavior of eriodictyol and fustin flavonoid compounds – A DFT study. AIP Conference Proceedings, 2018, , .	0.4	1
211	On the nexus between atom probe microscopy and density functional theory simulations. Materials Characterization, 2018, 146, 347-358.	4.4	19
213	Transferable Dynamic Molecular Charge Assignment Using Deep Neural Networks. Journal of Chemical Theory and Computation, 2018, 14, 4687-4698.	5.3	81

#	Article	IF	CITATIONS
214	Anisotropy of the Complex Permittivity of the Kagome-Staircase Compounds Co3V2O8 and Ni3V2O8: Experiment and Ab Initio Calculations. Journal of Experimental and Theoretical Physics, 2018, 126, 779-783.	0.9	1
215	Influence of Dislocations in Transition Metal Oxides on Selected Physical and Chemical Properties. Crystals, 2018, 8, 241.	2.2	54
216	Synergy between Experimental and Theoretical Results of Some Reactions of Annelated 1,3-Azaphospholes. Molecules, 2018, 23, 1283.	3.8	3
217	How accurate are static polarizability predictions from density functional theory? An assessment over 132 species at equilibrium geometry. Physical Chemistry Chemical Physics, 2018, 20, 19800-19810.	2.8	94
218	Hidden gapless states during thermal transformations of preorganized zinc alkoxides to zinc oxide nanocrystals. Materials Horizons, 2018, 5, 905-911.	12,2	11
219	First-principles study of polarization and piezoelectric properties of PbZrO3. AIP Conference Proceedings, 2018, , .	0.4	2
220	A multiscale model of the effect of Ir thickness on the static and dynamic properties of Fe/Ir/Fe films. Scientific Reports, 2018, 8, 3879.	3.3	1
221	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. Journal of Chemical Physics, 2018, 148, 171102.	3.0	20
222	Optical Transitions from Core d Levels of Gallium Arsenide. Physics of the Solid State, 2018, 60, 481-486.	0.6	1
223	Adsorption of Surfactants on α-Fe ₂ O ₃ (0001): A Density Functional Theory Study. Journal of Physical Chemistry C, 2018, 122, 20817-20826.	3.1	39
224	Hybrid Parallelization and Performance Optimization of the FLEUR Code: New Possibilities for All-Electron Density Functional Theory. Lecture Notes in Computer Science, 2018, , 735-748.	1.3	2
225	Accurate computation of X-ray absorption spectra with ionization potential optimized global hybrid functional. Journal of Chemical Physics, 2018, 149, 064111.	3.0	21
226	Many-body renormalization of forces in <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mi>f</mml:mi></mml:math> -electron materials. Physical Review B, 2018, 98, .	3.2	20
227	Molecular Modelling for Reactor Design. Annual Review of Chemical and Biomolecular Engineering, 2018, 9, 201-227.	6.8	31
228	Stability of FeVO ₄ under Pressure: An X-ray Diffraction and First-Principles Study. Inorganic Chemistry, 2018, 57, 7860-7876.	4.0	27
229	Combining theory and experiment in lithium–sulfur batteries: Current progress and future perspectives. Materials Today, 2019, 22, 142-158.	14.2	301
230	Direct observation of Eu atoms in AlN lattice and the firstâ€principles simulations. Journal of the American Ceramic Society, 2019, 102, 310-319.	3.8	20
231	Perdew-Zunger self-interaction correction: How wrong for uniform densities and large- <i>Z</i> atoms?. Journal of Chemical Physics, 2019, 150, 174106.	3.0	35

#	Article	IF	CITATIONS
232	Effect of Cu doping on microstructure and thermal stability of Ge2Sb2Te5 thin film. Applied Physics A: Materials Science and Processing, 2019, 125, 1.	2.3	8
233	Tight-Binding Model. Springer Theses, 2019, , 13-33.	0.1	0
234	Influences of spin-orbit coupling on Fermi surfaces and Dirac cones in ferroelectriclike polar metals. Physical Review B, 2019, 99, .	3.2	6
235	On combining the conductor-like screening model and optimally tuned range-separated hybrid density functionals. Journal of Chemical Physics, 2019, 150, 174117.	3.0	9
236	A first-principles roadmap and limits to design efficient supercapacitor electrode materials. Physical Chemistry Chemical Physics, 2019, 21, 17494-17511.	2.8	39
237	Efficient synthesis, spectroscopic characterization and DFT based studies of novel 1-amide 4-sulfonamide-1,2,3-triazole derivatives. Journal of Molecular Structure, 2019, 1197, 164-170.	3.6	14
238	Characteristics of carbon-expanded \hat{l}_{\pm} phase layer on AISI 431 stainless steel using experimental and fist-principles calculation methods. Surface and Coatings Technology, 2019, 375, 66-73.	4.8	7
239	First-principles study of Ni adatom migration on graphene with vacancies. RSC Advances, 2019, 9, 18823-18834.	3.6	7
240	How To Extract Quantitative Information on Electronic Transitions from the Density Functional Theory "Black Box― Journal of Chemical Theory and Computation, 2019, 15, 4915-4923.	5.3	9
241	Ab Initio Study of the Interface of the Solid-State Electrolyte Li ₉ N ₂ Cl ₃ Âwith a Li-Metal Electrode. Journal of the Electrochemical Society, 2019, 166, A2048-A2057.	2.9	19
242	A Reactionâ€Induced Localization of Spin Density Enables Thermal Câ^'H Bond Activation of Methane by Pristine FeC ₄ ⁺ . Chemistry - A European Journal, 2019, 25, 12940-12945.	3.3	22
243	Density-Driven Correlations in Many-Electron Ensembles: Theory and Application for Excited States. Physical Review Letters, 2019, 123, 016401.	7.8	28
244	New organic molecular based on Bis-Dipolar Diphenylamino-EndcappedOligo Aryl Fluorene Application for organic solar cells. Materials Today: Proceedings, 2019, 13, 1178-1187.	1.8	9
246	X-Ray Physics. , 2019, , 23-70.		0
247	Imaging Physics. , 2019, , 71-198.		0
248	X-Ray Focusing Optics. , 2019, , 199-240.		1
249	X-Ray Microscope Systems. , 2019, , 241-258.		0
250	X-Ray Spectromicroscopy., 2019, , 350-389.		0

#	Article	IF	Citations
251	Coherent Imaging. , 2019, , 390-456.		0
252	Radiation Damage and Cryo Microscopy. , 2019, , 457-495.		1
253	Applications, and Future Prospects. , 2019, , 496-514.		0
256	Relevance of the Pauli kinetic energy density for semilocal functionals. Physical Review B, 2019, 100, .	3.2	38
257	X-Ray Microscopes: a Short Introduction. , 2019, , 1-4.		0
258	A Bit of History. , 2019, , 5-22.		0
259	X-Ray Microscope Instrumentation. , 2019, , 259-320.		0
260	X-Ray Tomography. , 2019, , 321-349.		1
261	Atom-projected and angular momentum resolved density of states in the ONETEP code. Electronic Structure, 2019, 1, 035002.	2.8	7
262	Locally self-consistent embedding approach for disordered electronic systems. Physical Review B, 2019, 100, .	3.2	1
263	Thermodynamics of graphite intercalation binary alloys of Li-Na, Na-K, and Li-K from van der Waals density functionals. Journal of Solid State Electrochemistry, 2019, 23, 2825-2834.	2.5	2
264	Efficiency of free auxiliary models in describing interacting fermions: From the Kohn-Sham model to the optimal entanglement model. Physical Review B, 2019, 100, .	3.2	1
265	Current-induced spin-orbit torques in ferromagnetic and antiferromagnetic systems. Reviews of Modern Physics, $2019, 91, \ldots$	45.6	899
266	Enthalpies of formation of the benzyloxyl, benzylperoxyl, hydroxyphenyl radicals and related species on the potential energy surface for the reaction of toluene with the hydroxyl radical. Theoretical Chemistry Accounts, 2019, 138, 1.	1.4	3
267	Hohenberg–Kohn Theorems for Interactions, Spin and Temperature. Journal of Statistical Physics, 2019, 177, 415-437.	1.2	6
268	Understanding Carbamate Formation Reaction Thermochemistry of Amino Acids as Solvents for Postcombustion CO ₂ Capture. Journal of Physical Chemistry B, 2019, 123, 8433-8447.	2.6	13
269	Experimental and Theoretical Study of Surface-Enhanced Raman Spectra of Sulfadiazine Adsorbed on Nanoscale Gold Colloids. Journal of Physical Chemistry A, 2019, 123, 9199-9208.	2.5	12
270	Understanding the origin of bandgap problem in transition and post-transition metal oxides. Journal of Chemical Physics, 2019, 151, 124703.	3.0	8

#	Article	IF	CITATIONS
271	Phase-space modeling of solid-state plasmas. Reviews of Modern Plasma Physics, 2019, 3, 1.	4.1	20
272	Exact exchange-correlation potentials from ground-state electron densities. Nature Communications, 2019, 10, 4497.	12.8	54
273	Phase field crystal simulations of the kinetics of Ostwald ripening in two dimensions. Physical Review E, 2019, 99, 012803.	2.1	12
274	Functional renormalization-group calculation of the equation of state of one-dimensional uniform matter inspired by the Hohenberg-Kohn theorem. Physical Review C, 2019, 99, .	2.9	16
275	Reassessment of the Mechanisms of Thermal Câ^'H Bond Activation of Methane by Cationic Magnesium Oxides: A Critical Evaluation of the Suitability of Different Density Functionals. ChemPhysChem, 2019, 20, 1812-1821.	2.1	5
277	Ab initio path integral Monte Carlo approach to the static and dynamic density response of the uniform electron gas. Physical Review B, 2019, 99, .	3.2	53
278	A review on nonâ€relativistic, fully numerical electronic structure calculations on atoms and diatomic molecules. International Journal of Quantum Chemistry, 2019, 119, e25968.	2.0	45
279	The density response kernel, the Fukui function, and other response functions from the Kohn–Sham orbitals. Theoretical Chemistry Accounts, 2019, 138, 1.	1.4	4
280	Intermetalloid and Heterometallic Clusters Combining p-Block (Semi)Metals with d- or f-Block Metals. Chemical Reviews, 2019, 119, 8506-8554.	47.7	126
281	Temperature-dependent resistivity and anomalous Hall effect in NiMnSb from first principles. Physical Review B, 2019, 99, .	3.2	7
282	An alternative derivation of orbital-free density functional theory. Journal of Chemical Physics, 2019, 150, 204109.	3.0	6
283	High-throughput calculations of catalytic properties of bimetallic alloy surfaces. Scientific Data, 2019, 6, 76.	5.3	76
284	Current-constrained one-electron reduced density-matrix theory for non-equilibrium steady-state molecular conductivity. Physical Chemistry Chemical Physics, 2019, 21, 12620-12624.	2.8	4
286	Historical review of computer simulation of radiation effects in materials. Journal of Nuclear Materials, 2019, 520, 273-295.	2.7	121
287	Regularized SCAN functional. Journal of Chemical Physics, 2019, 150, 161101.	3.0	124
288	A critical assessment on the electron transport through dehydrogenated intrinsically conducting channels in graphane-graphene hybrids. Materials Research Express, 2019, 6, 085618.	1.6	1
289	The electrophilic descriptor. Computational and Theoretical Chemistry, 2019, 1157, 34-39.	2.5	27
290	Stretched or noded orbital densities and self-interaction correction in density functional theory. Journal of Chemical Physics, 2019, 150, 174102.	3.0	46

#	Article	IF	CITATIONS
291	Local Density Approximation for the Short-Range Exchange Free Energy Functional. ACS Omega, 2019, 4, 7675-7683.	3.5	16
292	Identifying Different Adsorption States of Methanol on ZnO(101\hat{\lambda}0); A Scanning Tunneling Microscopy and Density Functional Theory Study. Journal of Physical Chemistry C, 2019, 123, 9105-9111.	3.1	9
293	Theoretical study of the microhydration of 1â€chloro and 2â€chloro ethanol as a clue for their relative propensity toward dehalogenation. International Journal of Quantum Chemistry, 2019, 119, e25931.	2.0	5
294	Modeling Corrosion with First-Principles Electrochemical Phase Diagrams. Annual Review of Materials Research, 2019, 49, 53-77.	9.3	40
295	Deacetylation of per-acetatylated glycopyranosides: An overall pattern for acidic catalyzis. Chemical Physics Letters, 2019, 723, 123-127.	2.6	6
296	First-principles investigations on structural stability, elastic and electronic properties of Co ₇ M ₆ (M= W, Mo, Nb) µ phases. Molecular Simulation, 2019, 45, 752-758.	2.0	20
297	Basis Set Effects in the Description of the Cl-O Bond in ClO and XClO/ClOX Isomers (X = H, O, and Cl) Using DFT and CCSD(T) Methods. Journal of Chemistry, 2019, 2019, 1-23.	1.9	5
298	Organic piezoelectric materials: milestones and potential. NPG Asia Materials, 2019, 11, .	7.9	121
299	Bayesian inference of atomistic structure in functional materials. Npj Computational Materials, 2019, 5, .	8.7	81
300	Universal nature of different methods of obtaining the exact Kohn–Sham exchange-correlation potential for a given density. Journal of Physics B: Atomic, Molecular and Optical Physics, 2019, 52, 075007.	1.5	16
301	Managing uncertainty in data-derived densities to accelerate density functional theory. JPhys Materials, 2019, 2, 034001.	4.2	9
302	Removal of colorants from wastewater: A review on sources and treatment strategies. Journal of Industrial and Engineering Chemistry, 2019, 75, 1-19.	5.8	375
303	Dieter Cremer's contribution to the field of theoretical chemistry. International Journal of Quantum Chemistry, 2019, 119, e25849.	2.0	26
304	Well-behaved versus ill-behaved density functionals for single bond dissociation: Separating success from disaster functional by functional for stretched H2. Journal of Chemical Physics, 2019, 150, 094115.	3.0	25
305	$Ab-initio\$ description of excited states of 1D uniform matter with the Hohenbergae-"Kohn-theorem-inspired functional-renormalization-group method. Progress of Theoretical and Experimental Physics, 2019, 2019, .	6.6	13
306	Projection-Based Wavefunction-in-DFT Embedding. Accounts of Chemical Research, 2019, 52, 1359-1368.	15.6	88
307	Density-functional theory for plutonium. Advances in Physics, 2019, 68, 1-47.	14.4	45
308	Fully numerical Hartreeâ€Fock and density functional calculations. I. Atoms. International Journal of Quantum Chemistry, 2019, 119, e25945.	2.0	26

#	Article	IF	CITATIONS
309	Oxidation states of binary oxides from data analytics of the electronic structure. Computational Materials Science, 2019, 161, 403-414.	3.0	21
310	Modulating electronic coupling at the quantum dot/molecule interface by wavefunction engineering. Journal of Chemical Physics, 2019, 150, 124704.	3.0	2
311	Nanorod CoFe2O4 modified activated carbon as an efficient electrocatalyst to improve the performance of air cathode microbial fuel cell. Journal of Electroanalytical Chemistry, 2019, 840, 134-143.	3.8	19
312	Advances in Density-Functional Calculations for Materials Modeling. Annual Review of Materials Research, 2019, 49, 1-30.	9.3	87
313	Close Relationships between NMR <i>J</i> Coupling Alternation (JCA) and Molecular Properties of Carbon Chains. Journal of Chemical Theory and Computation, 2019, 15, 1605-1615.	5.3	4
314	Partial combination of composite strategy and the B3LYP functional for the calculation of enthalpies of formation. Journal of Molecular Modeling, 2019, 25, 62.	1.8	8
315	How To Make Your Computational Paper Interesting and Have It Published. Organometallics, 2019, 38, 603-605.	2.3	11
316	Efficient HF exchange evaluation through Fourier convolution in Cartesian grid for orbital-dependent density functionals. Journal of Chemical Physics, 2019, 150, 064104.	3.0	6
317	From DFT to machine learning: recent approaches to materials science–a review. JPhys Materials, 2019, 2, 032001.	4.2	385
318	Theoretical Calculations of the Multistep Reaction Mechanism Involved in Asparagine Pyrolysis Supported by Degree of Rate Control and Thermodynamic Control Analyses. Applied Sciences (Switzerland), 2019, 9, 4847.	2.5	3
319	Improvement of functionals in density functional theory by the inverse Kohn–Sham method and density functional perturbation theory. Journal of Physics B: Atomic, Molecular and Optical Physics, 2019, 52, 245003.	1.5	11
320	ElectroLens: Understanding Atomistic Simulations through Spatially-Resolved Visualization of High-Dimensional Features., 2019,,.		1
321	The influence of the grafted aryl groups on the solvation properties of the graphyne and graphdiyne - a MD study. Open Chemistry, 2019, 17, 703-710.	1.9	40
322	The static local field correction of the warm dense electron gas: An <i>ab initio</i> path integral Monte Carlo study and machine learning representation. Journal of Chemical Physics, 2019, 151, 194104.	3.0	64
323	Fast nonadiabatic dynamics of many-body quantum systems. Science Advances, 2019, 5, eaaw1634.	10.3	26
324	A step in the direction of resolving the paradox of Perdew-Zunger self-interaction correction. Journal of Chemical Physics, 2019, 151, 214108.	3.0	56
325	A two-density approach to the general many-body problem and a proof of principle for small atoms and molecules. Frontiers of Physics, 2019, 14, 1.	5.0	3
326	The Lewis electron-pair bonding model: the physical background, one century later. Nature Reviews Chemistry, 2019, 3, 35-47.	30.2	52

#	Article	IF	CITATIONS
327	Diverging Exchange Force and Form of the Exact Density Matrix Functional. Physical Review Letters, 2019, 122, 013001.	7.8	36
328	Synthesis, X-ray characterization, DFT studies and Hirshfeld surface analysis of new organic single crystal: 2-(4-Methoxyphenyl)-4-{[2'-(1H-tetrazol-5-yl)biphenyl-4-yl] methyl}-2,4-dihydro-3H-1,2,4-triazol-3-one (MTBT). Journal of Molecular Structure, 2019, 1179, 809-819.	3.6	19
329	Advantageous nearsightedness of many-body perturbation theory contrasted with Kohn-Sham density functional theory. Physical Review B, 2019 , 99 , .	3.2	10
330	Designing crystallization in phase-change materials for universal memory and neuro-inspired computing. Nature Reviews Materials, 2019, 4, 150-168.	48.7	572
331	Structural effect on the strength of non-covalent interactions in binary mixtures of benzyl amine and certain ethers through ultrasonic, FT-IR spectral and DFT studies at 303.15†K. Journal of Molecular Liquids, 2019, 277, 865-875.	4.9	10
332	The interplay and strength of the π⋯H F, C⋯H F, F⋯H F and F⋬H C hydrogen bonds upon the formation of multimolecular complexes based on C2H2⋬HF and C2H4⋬HF small dimers. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2019, 213, 438-455.	3.9	7
333	Polymorphs of ZnV ₂ O ₆ under Pressure: A First-Principle Investigation. Journal of Physical Chemistry C, 2019, 123, 3239-3253.	3.1	16
334	Low-energy heavy-ion reactions and the Skyrme effective interaction. Progress in Particle and Nuclear Physics, 2019, 104, 142-164.	14.4	59
335	Computational Approach to Molecular Catalysis by 3d Transition Metals: Challenges and Opportunities. Chemical Reviews, 2019, 119, 2453-2523.	47.7	260
336	Static polarizability and hyperpolarizability in atoms and molecules through a Cartesian-grid DFT. Theoretical Chemistry Accounts, 2019, 138, 1.	1.4	6
337	Voltammetric determination of chlorothalonil and its respective reduction mechanism studied by density functional theory. Journal of Solid State Electrochemistry, 2019, 23, 553-563.	2.5	6
338	Prebiotic chemistry and origins of life research with atomistic computer simulations. Physics of Life Reviews, 2020, 34-35, 105-135.	2.8	25
339	Theoretical study of the mechanism of 2,5-diketopiperazine formation during pyrolysis of proline. Molecular Physics, 2020, 118, .	1.7	8
340	sternheimerGW: A program for calculating <mml:math altimg="si24.svg" display="inline" id="d1e1442" xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mrow>G<mml:mi>W</mml:mi></mml:mrow></mml:math> quasiparticle band structures and spectral functions without unoccupied states. Computer Physics	7.5	12
341	Recent Progress in Lithium Niobate: Optical Damage, Defect Simulation, and Onâ€Chip Devices. Advanced Materials, 2020, 32, e1806452.	21.0	137
342	Quantum parameters based study of some heterocycles using density functional theory method: A comparative theoretical study. Journal of the Chinese Chemical Society, 2020, 67, 213-217.	1.4	8
343	Modeling Diffusion in Functional Materials: From Density Functional Theory to Artificial Intelligence. Advanced Functional Materials, 2020, 30, 1900778.	14.9	33
344	A theoretical investigation on the nucleophilic behavior of Meldrum's acid linked to experimental evidences. Chemical Physics Letters, 2020, 738, 136908.	2.6	3

#	Article	IF	Citations
345	Applications of Plasmon-Enhanced Nanocatalysis to Organic Transformations. Chemical Reviews, 2020, 120, 986-1041.	47.7	333
346	Machine learning models for the prediction of energy, forces, and stresses for Platinum. Computational Materials Science, 2020, 174, 109483.	3.0	17
347	Mechanism on The Disproportionating Synthesis of Dichlorodimethyl―silane by ZSMâ€5(5) Tj ETQq0 0 0 rgBT / 2020, 34, e5419.	Overlock : 3.5	10 Tf 50 667 ⁻ 5
348	Designing a bioremediator: mechanistic models guide cellular and molecular specialization. Current Opinion in Biotechnology, 2020, 62, 98-105.	6.6	16
349	Γ̂1¦: Solid state package allowing Bardeen–Cooper–Schrieffer and magnetic superstructure electronic states. Computer Physics Communications, 2020, 251, 107079.	7. 5	4
350	Stepwise Mechanism for the Bromination of Arenes by a Hypervalent lodine Reagent. Journal of Organic Chemistry, 2020, 85, 2142-2150.	3.2	27
351	Density functional theory calculations of the double gamma prime Ni3Ta phase under pressure: Structural, mechanical, and electronic properties. Journal of Physics and Chemistry of Solids, 2020, 138, 109248.	4.0	6
352	Role of Augmented Basis Sets and Quest for ab Initio Performance/Cost Alternative to Kohn–Sham Density Functional Theory. Journal of Physical Chemistry A, 2020, 124, 126-134.	2.5	9
353	Noncollinear Relativistic Two-Component X2C Calculations of Hyperfine Couplings Using Local Hybrid Functionals. Importance of the High-Density Coordinate Scaling Limit. Journal of Chemical Theory and Computation, 2020, 16, 314-325.	5.3	19
354	Modeling the Field Emission Enhancement Factor for Capped Carbon Nanotubes Using the Induced Electron Density. Journal of Chemical Information and Modeling, 2020, 60, 714-721.	5.4	10
355	Role of electronic correlation effect on charge ordering in \hat{I}^2 -V2OPO4. Computational Materials Science, 2020, 173, 109433.	3.0	0
356	Line-Graph Lattices: Euclidean and Non-Euclidean Flat Bands, and Implementations in Circuit Quantum Electrodynamics. Communications in Mathematical Physics, 2020, 376, 1909-1956.	2.2	58
357	How accurate is density functional theory in predicting spin density? An insight from the prediction of hyperfine coupling constants. Journal of Molecular Modeling, 2020, 26, 10.	1.8	18
358	Combining Embedded Mean-Field Theory with Linear-Scaling Density-Functional Theory. Journal of Chemical Theory and Computation, 2020, 16, 354-365.	5.3	3
359	Probing Hot Electron Behaviors by Surface-Enhanced Raman Spectroscopy. Cell Reports Physical Science, 2020, 1, 100184.	5.6	16
360	Perspective of computational modeling of nanomaterials. Frontiers of Nanoscience, 2020, , 1-3.	0.6	0
361	Recent advances of computational chemistry in organic solar cell research. Journal of Materials Chemistry C, 2020, 8, 15920-15939.	5.5	59
362	Magnesium and silicon in interstellar dust: X-ray overview. Astronomy and Astrophysics, 2020, 641, A149.	5.1	13

#	Article	IF	CITATIONS
363	Quantum Algorithms for Quantum Chemistry and Quantum Materials Science. Chemical Reviews, 2020, 120, 12685-12717.	47.7	311
364	Density functional and classical simulations of liquid and glassy selenium. Physical Review B, 2020, 102, .	3.2	4
365	Indole-3-carbaldehydes Arylhydrazones as Multisite C-Nucleophiles in the Reactions with Quinazoline. Russian Journal of General Chemistry, 2020, 90, 1601-1610.	0.8	2
366	High thermoelectric performance of half-Heusler compound BiBaK with intrinsically low lattice thermal conductivity. Journal of Physics Condensed Matter, 2020, 32, 425704.	1.8	7
367	The Seâ€ S/N interactions as a possible mechanism of Î-aminolevulinic acid dehydratase enzyme inhibition by organoselenium compounds: A computational study. Computational Toxicology, 2020, 15, 100127.	3.3	5
368	Catalytic function of ferric oxide and effect of water on the formation of sulfur trioxide. Journal of Environmental Management, 2020, 264, 110499.	7.8	6
369	Variational Multistate Density Functional Theory for a Balanced Treatment of Static and Dynamic Correlations. Journal of Chemical Theory and Computation, 2020, 16, 4912-4922.	5.3	7
370	The effect of N-heterocyclic carbene units on the absorption spectra of Fe(<scp>ii</scp>) complexes: a challenge for theory. Physical Chemistry Chemical Physics, 2020, 22, 27605-27616.	2.8	8
371	The Fermi–Löwdin self-interaction correction for ionization energies of organic molecules. Journal of Chemical Physics, 2020, 153, 184303.	3.0	12
372	The Pseudopotential Approach within Density-Functional Theory: The Case of Atomic Metallic Hydrogen. Condensed Matter, 2020, 5, 74.	1.8	0
373	Intramolecular Hydrogen Bonds in Tip-Functionalized Single-Walled Carbon Nanotubes as pH-Sensitive Gates. Journal of Physical Chemistry A, 2020, 124, 9542-9551.	2.5	6
374	Machine learning accurate exchange and correlation functionals of the electronic density. Nature Communications, 2020, 11 , 3509.	12.8	120
375	Electronic-structure methods for twisted moiré layers. Nature Reviews Materials, 2020, 5, 748-763.	48.7	142
376	Density functional theory calculations of the effect (CH2, CH3, NH3, NH2, OH, CN, NO2) subgroups on the electronic structure of biphenyl molecule. IOP Conference Series: Materials Science and Engineering, 2020, 871, 012067.	0.6	0
377	Scaling behavior of the momentum distribution of a quantum Coulomb system in a confining potential. Physical Review B, 2020, 102, .	3.2	0
378	Spatial density neural network force fields with first-principles level accuracy and application to thermal transport. Physical Review B, 2020, 102, .	3.2	20
379	Ce0.5La0.5Ni9Ge4 compound: Why is cerium valence not 3+?. Chinese Journal of Physics, 2020, 67, 473-481.	3.9	0
380	Unveiling the structural origin to control resistance drift in phase-change memory materials. Materials Today, 2020, 41, 156-176.	14.2	96

#	Article	IF	Citations
381	Ab initio calculations and a scratch test study of RF-magnetron sputter deposited hydroxyapatite and silicon-containing hydroxyapatite coatings. Surfaces and Interfaces, 2020, 21, 100727.	3.0	7
382	Using coarse-grained molecular dynamics to rationalize biomolecule solubilization mechanisms in ionic liquid-based colloidal systems. Physical Chemistry Chemical Physics, 2020, 22, 24771-24783.	2.8	9
383	Models and corrections: Range separation for electronic interactionâ€"Lessons from density functional theory. Journal of Chemical Physics, 2020, 153, 160901.	3.0	12
384	Dynamic properties of the warm dense electron gas based on abÂinitio path integral Monte Carlo simulations. Physical Review B, 2020, 102, .	3.2	42
385	Atomic shell structure from an orbital-free-related density-functional-theory Pauli potential. Physical Review A, 2020, 102, .	2.5	5
386	Localization in the SCAN meta-generalized gradient approximation functional leading to broken symmetry ground states for graphene and benzene. Physical Chemistry Chemical Physics, 2020, 22, 19585-19591.	2.8	8
387	Density Functional Theory: Foundations. , 2020, , 129-144.		0
388	Deriving the vibronic coupling constants of the cyclopentadienyl radical with density functional theory and GOWO. Journal of Chemical Physics, 2020, 153, 064303.	3.0	2
389	Nanoscale Modeling of Surface Phenomena in Aluminum Using Machine Learning Force Fields. Journal of Physical Chemistry C, 2020, 124, 22127-22136.	3.1	9
390	Excitation energies from thermally assisted-occupation density functional theory: Theory and computational implementation. Journal of Chemical Physics, 2020, 153, 084120.	3.0	10
391	Understanding the electrochemical oxidation of dyes on platinum and boron–doped diamond electrode surfaces: experimental and computational study. Journal of Solid State Electrochemistry, 2020, 24, 3245-3256.	2.5	16
392	Maple's Quantum Chemistry Package in the Chemistry Classroom. Journal of Chemical Education, 2020, 97, 3658-3666.	2.3	8
393	Tuning the Baird aromatic triplet-state energy of cyclooctatetraene to maximize the self-healing mechanism in organic fluorophores. Proceedings of the National Academy of Sciences of the United States of America, 2020, 117, 24305-24315.	7.1	35
394	Classical dynamical density functional theory: from fundamentals to applications. Advances in Physics, 2020, 69, 121-247.	14.4	126
395	Impact of phonon nonlocality on nanogap and nanolayer polar resonators. Physical Review B, 2020, 102, .	3.2	14
396	Molecular modeling and density functional theory calculation of the coordination behavior of 4,5-Dichloroimidazole with Cu(II) ion. Scientific African, 2020, 9, e00533.	1.5	5
397	Ensemble Density Functional Theory: Insight from the Fluctuation-Dissipation Theorem. Physical Review Letters, 2020, 125, 233001.	7.8	17
398	Calculation of the detonation state of HN3 with quantum accuracy. Journal of Chemical Physics, 2020, 153, 224102.	3.0	14

#	Article	IF	CITATIONS
399	Lithium Niobate Single Crystals and Powders Reviewedâ€"Part II. Crystals, 2020, 10, 990.	2.2	27
400	Multiscale Modeling of Defect Phenomena in Platinum Using Machine Learning of Force Fields. Jom, 2020, 72, 4346-4358.	1.9	5
401	Partitioning a Molecule into the Atomic Basins and the Resultant Atomic Charges from Quantum Chemical Topology Analysis of the Kohn–Sham Potential. Journal of Physical Chemistry A, 2020, 124, 5023-5032.	2.5	3
402	Metastability at Defective Metal Oxide Interfaces and Nanoconfined Structures. Advanced Materials Interfaces, 2020, 7, 1902090.	3.7	20
403	High-pressure characterization of multifunctional CrVO ₄ . Journal of Physics Condensed Matter, 2020, 32, 385403.	1.8	12
404	Reduced Density Matrix Functional Theory for Bosons. Physical Review Letters, 2020, 124, 180603.	7.8	23
405	Interface enhanced functionalities in oxide superlattices under mechanical and electric boundary conditions. Npj Computational Materials, 2020, 6, .	8.7	9
406	<i>Ab initio</i> path integral monte carlo simulation of the uniform electron gas in the high energy density regime. Plasma Physics and Controlled Fusion, 2020, 62, 075003.	2.1	28
407	Improvement of oxygen reduction capacity by activated carbon doped with broccoli-like Co-Ni2P in microbial fuel cells. Chemical Engineering Journal, 2020, 399, 125601.	12.7	16
408	Modeling temperature dependent and absolute carbamate stability constants of amines for CO2 capture. International Journal of Greenhouse Gas Control, 2020, 98, 103061.	4.6	10
409	Atom Classification Model for Total Energy Evaluation of Two-Dimensional Multicomponent Materials. Journal of Physical Chemistry A, 2020, 124, 4506-4511.	2.5	13
410	CP2K: An electronic structure and molecular dynamics software package - Quickstep: Efficient and accurate electronic structure calculations. Journal of Chemical Physics, 2020, 152, 194103.	3.0	1,371
411	Predicting the dynamic behavior of the mechanical properties of platinum with machine learning. Journal of Chemical Physics, 2020, 152, 224709.	3.0	4
412	Analysis of Electronic and Optical Properties of Pristine LiNbO3 Using First-Principle Calculations. , 2020, , .		1
413	DFT study of electronic and optical properties of nickel doped barium titanate nanostructures. AIP Conference Proceedings, 2020, , .	0.4	0
414	A step in the direction of resolving the paradox of Perdew–Zunger self-interaction correction. II. Gauge consistency of the energy density at three levels of approximation. Journal of Chemical Physics, 2020, 152, 214109.	3.0	23
415	Parallel Implementation of Density Functional Theory Methods in the Quantum Interaction Computational Kernel Program. Journal of Chemical Theory and Computation, 2020, 16, 4315-4326.	5.3	25
416	ONETEP + TOSCAM: Uniting Dynamical Mean Field Theory and Linear-Scaling Density Functional Theory. Journal of Chemical Theory and Computation, 2020, 16, 4899-4911.	5.3	5

#	Article	IF	Citations
417	Solid electrolyte interphase formation between the Li _{0.29} La _{0.57} TiO ₃ solid-state electrolyte and a Li-metal anode: an <i>ab initio</i> molecular dynamics study. RSC Advances, 2020, 10, 9000-9015.	3.6	12
418	Data-Based Methods for Materials Design and Discovery: Basic Ideas and General Methods. Synthesis Lectures on Materials and Optics, 2020, 1, 1-188.	0.2	6
419	Electronic Structure and Optical Properties of the FeAl2 Compound. Physics of the Solid State, 2020, 62, 106-109.	0.6	1
422	Electrons and Band Theory: Formalism in the One-Electron Approximation. , 2020, , 33-62.		0
423	Electrons and Band Theory: Methods of Energy-Band Calculations. , 2020, , 63-114.		0
424	Electrons and Band Theory: Effects of Spin–Orbit Interactions. , 2020, , 115-145.		0
425	Linear Response and the Dielectric Function. , 2020, , 146-165.		0
426	Phonons and Lattice Dynamics. , 2020, , 166-199.		0
427	Dimensionality, Susceptibility, and Instabilities. , 2020, , 200-216.		0
428	Topological Aspects of Condensed Matter Physics: A Historical Perspective. , 2020, , 219-223.		0
429	Topological Preliminaries. , 2020, , 224-253.		0
430	Berry-ology. , 2020, , 254-285.		0
431	Topological Aspects of Insulator Band Structure and Early Discoveries. , 2020, , 286-330.		0
432	Dirac Materials and Dirac Fermions. , 2020, , 331-372.		0
433	Many-Body Physics and Second Quantization. , 2020, , 375-408.		0
434	The Interacting Electron Gas. , 2020, , 409-424.		0
435	Green Functions for Many-Body Systems and Feynman Diagrams. , 2020, , 425-517.		0
436	Path Integrals. , 2020, , 518-541.		0

#	Article	IF	CITATIONS
437	Boson Systems: Bose–Einstein Condensation and Superfluidity. , 2020, , 542-583.		0
438	Landau Fermi Liquid Theory. , 2020, , 584-607.		O
439	Non-Fermi Liquids, the Luttinger Liquid, and Bosonization. , 2020, , 608-643.		0
440	Electron–Phonon Interactions. , 2020, , 644-665.		O
441	Microscopic Theory of Conventional Superconductivity., 2020,, 666-710.		0
442	Quantum Theory of Magnetism: Exchange Coupling Mechanisms. , 2020, , 711-744.		0
443	Quantum Theory of Magnetism: Magnetic Insulator Ground States and Spin-Wave Excitations. , 2020, , 745-768.		0
444	Quantum Theory of Magnetism: Itinerant-Electron Systems and the Kondo Effect., 2020,, 769-807.		0
445	The Basics of Covalent Bonding in Terms of Energy and Dynamics. Molecules, 2020, 25, 2667.	3.8	18
446	Exploiting chemistry and molecular systems for quantum information science. Nature Reviews Chemistry, 2020, 4, 490-504.	30.2	247
447	Insights into the photoprotection mechanism of the UV filter homosalate. Physical Chemistry Chemical Physics, 2020, 22, 15509-15519.	2.8	26
448	Electronic and optical properties of nickel doped potassium titanate nanostructures: A DFT study. AIP Conference Proceedings, 2020, , .	0.4	0
449	Homogeneous electron gas in arbitrary dimensions. Physical Review B, 2020, 102, .	3.2	2
450	Examination of high-throughput hybrid calculations using coarser reciprocal space meshes. Current Applied Physics, 2020, 20, 379-383.	2.4	10
452	Computational and Experimental Analysis of Carbon Functional Nanomaterials., 2020,, 269-311.		0
453	Vibrational dynamics in lead halide hybrid perovskites investigated by Raman spectroscopy. Physical Chemistry Chemical Physics, 2020, 22, 5604-5614.	2.8	61
454	Robust, Accurate, and Efficient: Quantum Embedding Using the Huzinaga Level-Shift Projection Operator for Complex Systems. Journal of Chemical Theory and Computation, 2020, 16, 2284-2295.	5.3	14
455	Asymptotic Behavior of the Exchangeâ€Correlation Energy Density and the Kohnâ€Sham Potential in Density Functional Theory: Exact Results and Strategy for Approximations. Israel Journal of Chemistry, 2020, 60, 805-822.	2.3	14

#	Article	IF	CITATIONS
456	Invited Review: Modern Methods for Accurately Simulating the Terahertz Spectra of Solids. Journal of Infrared, Millimeter, and Terahertz Waves, 2020, 41, 491-528.	2.2	35
457	Lattice dynamics of palladium in the presence of electronic correlations. Physical Review B, 2020, 101, .	3.2	3
458	Second-Harmonic Generation from a Quantum Emitter Coupled to a Metallic Nanoantenna. ACS Photonics, 2020, 7, 701-713.	6.6	12
459	Unique continuation for the magnetic Schr $ ilde{A}$ qdinger equation. International Journal of Quantum Chemistry, 2020, 120, e26149.	2.0	3
460	Strongly coupled electron liquid: $\langle i \rangle$ Ab initio $\langle i \rangle$ path integral Monte Carlo simulations and dielectric theories. Physical Review B, 2020, 101, .	3.2	38
461	Effect of external pressure on the structural stability, electronic structure, band gap engineering and optical properties of LiNbO3: An ab-initio calculation. Materials Today Communications, 2020, 23, 100919.	1.9	25
462	Vibrational Raman spectroscopy on adsorbate-induced low-dimensional surface structures. Surface Science Reports, 2020, 75, 100480.	7.2	4
463	Theoretical and experimental study of the influence of cation–Eriochrome complexes on the BDD anodic oxidation of Eriochrome Black T solutions. Electrochemistry Communications, 2020, 112, 106668.	4.7	13
464	Novel carbohydrazones including 5-substituted isatin: Synthesis, characterization, and quantum-chemical studies on the relationship between electronic and antioxidant properties. Journal of Physics and Chemistry of Solids, 2020, 140, 109362.	4.0	16
465	Evaluation of Polaron Transport in Solids from Firstâ€principles. Israel Journal of Chemistry, 2020, 60, 768-786.	2.3	41
466	A Quadratic Pair Atomic Resolution of the Identity Based SOS-AO-MP2 Algorithm Using Slater Type Orbitals. Journal of Chemical Theory and Computation, 2020, 16, 875-891.	5. 3	23
467	Orbital localization error of density functional theory in shear properties of vanadium and niobium. Journal of Chemical Physics, 2020, 152, 024118.	3.0	8
468	Modified Density Functional Dispersion Correction for Inorganic Layered MFX Compounds (M = Ca, Sr,) Tj ETQq0	0.0 rgBT / 2.5	'Oyerlock 10
469	Harnessing aromaticity to design of phosphazene and ylidophosphorane superbases: A theoretical study. Computational and Theoretical Chemistry, 2020, 1174, 112714.	2.5	6
470	Bayesian Optimization for Calibrating and Selecting Hybrid-Density Functional Models. Journal of Physical Chemistry A, 2020, 124, 4053-4061.	2.5	107
471	Stability, geometry and electronic properties of BHn(n  =  0 to 3) radicals on the Si{0 0â€ from first-principles. Journal of Physics Condensed Matter, 2020, 32, 235201.	‰1}3â€% 1.8	â <u>≨</u> ‰Ã—â€
472	Hybrid functionals with systemâ€dependent parameters: Conceptual foundations and methodological developments. Wiley Interdisciplinary Reviews: Computational Molecular Science, 2020, 10, e1476.	14.6	7
473	Ab initio typical medium theory of substitutional disorder. Physical Review B, 2020, 101, .	3 . 2	5

#	Article	IF	CITATIONS
474	Density Functional Theory in the Prediction of Mutagenicity: A Perspective. Chemical Research in Toxicology, 2021, 34, 179-188.	3.3	15
475	A Roadmap for Production of Cement and Concrete with Low-CO2 Emissions. Waste and Biomass Valorization, 2021, 12, 4745-4775.	3.4	21
476	Effects of KF and RbF treatments on Cu(In,Ga)Se2-based solar cells: A combined photoelectron spectroscopy and DFT study. Applied Surface Science, 2021, 538, 148085.	6.1	7
477	Optical properties of organosilicon compounds containing sigma-electron delocalization by quasiparticle self-consistent GW calculations. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2021, 245, 118939.	3.9	9
478	Fixation stability of glass matrix co-existent with crystal phases for heavy metals formed by high-temperature vitrification. Environmental Science and Pollution Research, 2021, 28, 13660-13670.	5.3	7
479	Quantum Information and Algorithms for Correlated Quantum Matter. Chemical Reviews, 2021, 121, 3061-3120.	47.7	67
480	Angle, Spin, and Depth Resolved Photoelectron Spectroscopy on Quantum Materials. Chemical Reviews, 2021, 121, 2816-2856.	47.7	16
481	<scp>Schrödinger–Pauli</scp> theory of electrons: New perspectives. International Journal of Quantum Chemistry, 2021, 121, e26556.	2.0	11
482	Understanding the Photoexcitation of Room Temperature Ionic Liquids. ChemistryOpen, 2021, 10, 72-82.	1.9	1
483	Atomistic modeling of laser-related phenomena. , 2021, , 79-136.		0
484	Sonogashira cross-coupling reactions of 5-(benzothiazol-2-yl)-1-(4-iodophenyl)-3-phenyl-6-vinyl(phenyl)verdazyls: synthetic and theoretical aspects. Chemistry of Heterocyclic Compounds, 2021, 57, 40-48.	1.2	2
485	Local self-interaction correction method with a simple scaling factor. Physical Chemistry Chemical Physics, 2021, 23, 2406-2418.	2.8	14
486	Structural and elastic properties of binary semiconductors from energy gaps. Applied Physics A: Materials Science and Processing, 2021, 127, 1.	2.3	2
487	Mandrel degradation model of combined fast and slow processes. High Power Laser Science and Engineering, 2021, 9, .	4.6	5
488	Exact exchange-correlation potentials for calculating the fundamental gap with a fixed number of electrons. Physical Review A, 2021, 103, .	2.5	3
489	Uncomputability of phase diagrams. Nature Communications, 2021, 12, 452.	12.8	7
490	Anomeric effect, hyperconjugation and electrostatics: lessons from complexity in a classic stereoelectronic phenomenon. Chemical Society Reviews, 2021, 50, 10212-10252.	38.1	78
491	Meta-Local Density Functionals: A New Rung on Jacob's Ladder. Journal of Chemical Theory and Computation, 2021, 17, 943-948.	5.3	4

#	Article	IF	CITATIONS
492	Strategy and Future Prospects to Develop Room-Temperature-Recoverable NO2 Gas Sensor Based on Two-Dimensional Molybdenum Disulfide. Nano-Micro Letters, 2021, 13, 38.	27.0	103
493	How many shades of grey? On the proximity of density functional approximation to ab initio method via calculations of electric multipole moments. Journal of Physics: Conference Series, 2021, 1730, 012126.	0.4	0
494	Computational approaches to dissociative chemisorption on metals: towards chemical accuracy. Physical Chemistry Chemical Physics, 2021, 23, 8962-9048.	2.8	47
495	<i>Ab initio</i> electronic density in solids by many-body plane-wave auxiliary-field quantum Monte Carlo calculations. Physical Review B, 2021, 103, .	3.2	8
496	Understanding the electro-catalytic effect of benzene ring substitution on the electrochemical oxidation of aniline and its derivatives using BDD anode: Cyclic voltammetry, bulk electrolysis and theoretical calculations. Electrochimica Acta, 2021, 369, 137688.	5.2	12
498	Interfaces between crystalline Si and amorphous B: Interfacial interactions and charge barriers. Physical Review B, 2021, 103, .	3.2	4
499	Sulfur Molecules in Space by X-rays: A Computational Study. ACS Earth and Space Chemistry, 2021, 5, 436-448.	2.7	6
500	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. Journal of Chemical Physics, 2021, 154, 074109.	3.0	15
501	From Kohnâ€"Sham to Many-Electron Energies via Step Structures in the Exchange-Correlation Potential. Journal of Chemical Theory and Computation, 2021, 17, 1390-1407.	5. 3	12
502	Implementation of Perdew–Zunger self-interaction correction in real space using Fermi–Löwdin orbitals. Journal of Chemical Physics, 2021, 154, 084112.	3.0	7
503	Describing adsorption of benzene, thiophene, and xenon on coinage metals by using the Zaremba–Kohn theory-based model. Journal of Chemical Physics, 2021, 154, 124705.	3.0	4
504	Diffusion, relaxation, and aging of liquid and amorphous selenium. Physical Review B, 2021, 103, .	3.2	6
505	Overcoming finite-size effects in electronic structure simulations at extreme conditions. Journal of Chemical Physics, 2021, 154, 144103.	3.0	24
506	Self-Interaction-Corrected Random Phase Approximation. Journal of Chemical Theory and Computation, 2021, 17, 2107-2115.	5.3	2
507	Electronic, vibrational and optical properties of two-electron atoms and ions trapped in small fullerene-like cages. Journal of Physics B: Atomic, Molecular and Optical Physics, 2021, 54, 065101.	1.5	0
508	Magnetic Compton profiles of Ni beyond the one-particle picture: Numerically exact and perturbative solvers of dynamical mean-field theory. Physical Review B, 2021, 103, .	3.2	3
509	Treecode-accelerated Green iteration for Kohn-Sham density functional theory. Journal of Computational Physics, 2021, 430, 110101.	3.8	3
510	Atomistic Modeling of PEDOT:PSS Complexes I: DFT Benchmarking. Macromolecules, 2021, 54, 3634-3646.	4.8	14

#	Article	IF	CITATIONS
511	Measuring Density Functional Parameters from Electron Diffraction Patterns. Physical Review Letters, 2021, 126, 176402.	7.8	2
512	Linear scaling quantum transport methodologies. Physics Reports, 2021, 903, 1-69.	25.6	46
513	Computational Approaches: An Underutilized Tool in the Quest to Elucidate Radical SAM Dynamics. Molecules, 2021, 26, 2590.	3.8	5
514	Analytical representation of the local field correction of the uniform electron gas within the effective static approximation. Physical Review B, 2021, 103, .	3.2	31
515	Optical-electronic performance and mechanism investigation of dihydroindolocarbazole-based organic dyes for DSSCs. Results in Physics, 2021, 23, 103939.	4.1	8
516	Molecular Dynamicsâ€"From Small Molecules to Macromolecules. International Journal of Molecular Sciences, 2021, 22, 3761.	4.1	17
517	Fermi-LÃ \P wdin-orbital self-interaction correction using the optimized-effective-potential method within the Krieger-Li-lafrate approximation. Physical Review A, 2021, 103, .	2.5	14
518	Engineering analog quantum chemistry Hamiltonians using cold atoms in optical lattices. Physical Review A, 2021, 103, .	2.5	3
519	Concentration discontinuity of alkalies at high pressures. Physics Letters, Section A: General, Atomic and Solid State Physics, 2021, 395, 127207.	2.1	5
520	Investigations of the intrinsic corrosion and hydrogen susceptibility of metals and alloys using density functional theory. Corrosion Reviews, 2021, 39, 177-209.	2.0	10
521	Discovering and understanding materials through computation. Nature Materials, 2021, 20, 728-735.	27.5	60
522	Introducing LibXC into GAMESS (US). Mendeleev Communications, 2021, 31, 302-305.	1.6	2
523	Long-Time Behaviour of Time-Dependent Density Functional Theory. Archive for Rational Mechanics and Analysis, 2021, 241, 447-473.	2.4	3
524	Introducing LibXC into GAMESS (US). Mendeleev Communications, 2021, 31, 302-305.	1.6	0
525	Resource estimate for quantum many-body ground-state preparation on a quantum computer. Physical Review A, 2021, 103, .	2.5	13
526	Vibrational spectroscopy and phononâ€related properties of monoclinic GABA, a nonâ€proteinogenic inhibitory neurotransmitter amino acid. Journal of Raman Spectroscopy, 2021, 52, 1294-1307.	2.5	1
527	Band structures of RE ₂ O ₃ :Eu (RE = Lu, Y, Sc) from perspective of spin-polarized quasi-particle approximation. Modelling and Simulation in Materials Science and Engineering, 2021, 29, 065002.	2.0	3
528	Dynamical correlation energy of metals in large basis sets from downfolding and composite approaches. Journal of Chemical Physics, 2021, 154, 211105.	3.0	13

#	Article	IF	CITATIONS
529	From Electronegativity towards Reactivityâ€"Searching for a Measure of Atomic Reactivity. Molecules, 2021, 26, 3680.	3.8	4
530	Coupled-cluster method for the electronic structure and spectroscopic constants in halohydride cations with spin–orbit coupling. Chemical Physics Letters, 2021, 773, 138590.	2.6	0
531	Opportunities given by density functional theory in pathological calcifications. Comptes Rendus Chimie, 2022, 25, 209-218.	0.5	7
532	Machine Learning Kinetic Energy Functional for a One-Dimensional Periodic System. Chinese Physics Letters, 2021, 38, 050701.	3.3	3
533	Process and engineering aspects of carbon capture by ionic liquids. Journal of CO2 Utilization, 2021, 48, 101507.	6.8	14
534	A density functional theory (DFT) investigation of how small molecules and atmospheric pollutants relevant to art conservation adsorb on kaolinite. Applied Clay Science, 2021, 206, 106075.	5.2	11
535	Easy Access to Energy Fluctuations in Nonequilibrium Quantum Many-Body Systems. Physical Review Letters, 2021, 127, 030602.	7.8	6
536	First-Principles Study on the Electronic Properties of PDPP-Based Conjugated Polymer via Density Functional Theory. Journal of Physical Chemistry B, 2021, 125, 8953-8964.	2.6	7
537	Current progress of Pt-based ORR electrocatalysts for PEMFCs: An integrated view combining theory and experiment. Materials Today Physics, 2021, 19, 100406.	6.0	65
538	Strategies for the construction of machine-learning potentials for accurate and efficient atomic-scale simulations. Machine Learning: Science and Technology, 2021, 2, 031001.	5.0	42
539	Projector-Based Quantum Embedding for Molecular Systems: An Investigation of Three Partitioning Approaches. Journal of Physical Chemistry A, 2021, 125, 6384-6393.	2.5	9
540	Electrochemistry from first-principles in the grand canonical ensemble. Journal of Chemical Physics, 2021, 155, 024114.	3.0	11
541	Accurate density functional made more versatile. Journal of Chemical Physics, 2021, 155, 024103.	3.0	15
542	In Search of an Efficient Complexing Agent for Oxalates and Phosphates: A Quantum Chemical Study. Nanomaterials, 2021, 11, 1763.	4.1	8
543	Order- <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"> <mml:mi>N</mml:mi></mml:math> orbital-free density-functional calculations with machine learning of functional derivatives for semiconductors and metals. Physical Review Research, 2021, 3, .	3.6	16
544	Self-interaction-corrected Kohn–Sham effective potentials using the density-consistent effective potential method. Journal of Chemical Physics, 2021, 155, 064109.	3.0	8
545	Systematic Investigation of Error Distribution in Machine Learning Algorithms Applied to the Quantum-Chemistry QM9 Data Set Using the Bias and Variance Decomposition. Journal of Chemical Information and Modeling, 2021, 61, 4210-4223.	5.4	6
546	Nonlinear density response from imaginary-time correlation functions: <i>Ab initio</i> path integral Monte Carlo simulations of the warm dense electron gas. Journal of Chemical Physics, 2021, 155, 054110.	3.0	26

#	Article	IF	CITATIONS
547	Rangeâ€separated multiconfigurational density functional theory methods. Wiley Interdisciplinary Reviews: Computational Molecular Science, 0, , e1566.	14.6	9
548	Double excitations in molecules from ensemble density functionals: Theory and approximations. Physical Review A, 2021, 104, .	2.5	10
549	Common workflows for computing material properties using different quantum engines. Npj Computational Materials, 2021, 7, .	8.7	10
550	Melt-quenched and as-deposited structures of amorphous selenium: a density functional/ molecular dynamics comparison. Journal of Physics Condensed Matter, 2021, 33, 445401.	1.8	2
551	Precipitation during creep in magnesium–aluminum alloys. Continuum Mechanics and Thermodynamics, 2021, 33, 2363-2374.	2.2	0
552	Structural, elastic, vibrational, electronic and optical properties of SmFeO3 using density functional theory. Physica B: Condensed Matter, 2021, 615, 413061.	2.7	14
553	Gaussian Process Regression for Materials and Molecules. Chemical Reviews, 2021, 121, 10073-10141.	47.7	384
554	Rapid screening of high-throughput ground state predictions. Calphad: Computer Coupling of Phase Diagrams and Thermochemistry, 2021, 74, 102306.	1.6	2
555	Electronic Exciton–Plasmon Coupling in a Nanocavity Beyond the Electromagnetic Interaction Picture. Nano Letters, 2021, 21, 8466-8473.	9.1	8
556	A self-consistent systematic optimisation of range-separated hybrid functionals from first principles. Molecular Physics, 0, , .	1.7	3
557	<i>Ab initio</i> study of lattice dynamics of group IV semiconductors using pseudohybrid functionals for extended Hubbard interactions. Physical Review B, 2021, 104, .	3.2	9
558	Magnetic properties and electronic structure of Mn-Al alloys in the \hat{l}^2 -Mn structure. Journal of Magnetism and Magnetic Materials, 2022, 542, 168600.	2.3	4
559	On the inclusion of one double within CIS and TDDFT. Journal of Chemical Physics, 2021, 155, 154105.	3.0	7
560	Simulating quantum materials with digital quantum computers. Quantum Science and Technology, 2021, 6, 043002.	5.8	32
561	Symmetry restoration in mean-field approaches. Journal of Physics G: Nuclear and Particle Physics, 2021, 48, 123001.	3.6	62
562	Computational Materials Insights Into Solid-State Multiqubit Systems. PRX Quantum, 2021, 2, .	9.2	3
563	Baltimore SCIART: A Fully Virtual Undergraduate Research Experience at the Interface of Computational Chemistry and Art. Journal of Chemical Education, 0, , .	2.3	1
564	Machine learning universal bosonic functionals. Physical Review Research, 2021, 3, .	3.6	11

#	Article	lF	Citations
565	Mechanisms, challenges, and opportunities of dual Ni/ <scp>photoredoxâ€catalyzed</scp> C(sp ²)–C(sp ³) <scp>crossâ€couplings</scp> . Wiley Interdisciplinary Reviews: Computational Molecular Science, 2022, 12, e1573.	14.6	20
566	Highly accurate machine learning model for kinetic energy density functional. Physics Letters, Section A: General, Atomic and Solid State Physics, 2021, 414, 127621.	2.1	8
567	VASPKIT: A user-friendly interface facilitating high-throughput computing and analysis using VASP code. Computer Physics Communications, 2021, 267, 108033.	7.5	2,308
568	Fe2GeS4 (010) surface oxidation mechanism and potential application of the oxidized surface in gas sensing: A first-principles study. Journal of Alloys and Compounds, 2021, 888, 161532.	5. 5	2
569	Theoretical studies of dimers and properties of the corrosion inhibitor profile for semicarbazones and thiosemicarbazones. Journal of Molecular Liquids, 2021, 343, 117660.	4.9	6
570	Computing Eigenspaces With Low Rank Constraints. SIAM Journal of Scientific Computing, 2021, 43, A586-A608.	2.8	0
571	Bypassing the computational bottleneck of quantum-embedding theories for strong electron correlations with machine learning. Physical Review Research, 2021, 3, .	3.6	5
572	Problems of Visualization and 3d Modeling in Chemistry: Analysis of Electronodonor Properties and Spatial Complex-Forming Structure of the Obtained Sulfocationite. Advances in Intelligent Systems and Computing, 2021, , 262-271.	0.6	0
573	How well do self-interaction corrections repair the overestimation of static polarizabilities in density functional calculations?. Physical Chemistry Chemical Physics, 2021, 23, 18678-18685.	2.8	14
574	Kohn-Sham Equations as Regularizer: Building Prior Knowledge into Machine-Learned Physics. Physical Review Letters, 2021, 126, 036401.	7.8	89
575	Photovoltaic Materials Design by Computational Studies: Metal Sulfides. , 2020, , 123-138.		2
576	Density Functional Calculations. , 2016, , 483-563.		1
577	Review on Simulation Models for Materials and Biomolecular Study and Design., 2017,, 373-408.		3
581	Efficient training of ANN potentials by including atomic forces via Taylor expansion and application to water and a transition-metal oxide. Npj Computational Materials, 2020, 6, .	8.7	40
582	Machine-guided representation for accurate graph-based molecular machine learning. Physical Chemistry Chemical Physics, 2020, 22, 18526-18535.	2.8	25
583	Entangled light–matter interactions and spectroscopy. Journal of Materials Chemistry C, 2020, 8, 10732-10741.	5.5	34
584	Large scale and linear scaling DFT with the CONQUEST code. Journal of Chemical Physics, 2020, 152, 164112.	3.0	55
585	Insights from the density functional performance of water and water–solid interactions: SCAN in relation to other meta-GGAs. Journal of Chemical Physics, 2020, 153, 214116.	3.0	14

#	Article	IF	CITATIONS
586	Model nuclear energy density functionals derived from ab initio calculations. Journal of Physics G: Nuclear and Particle Physics, 2020, 47, 085107.	3.6	13
587	Virtual screening of nitrogen-, phosphorous- and halide-containing materials as p-type transparent conductors. JPhys Materials, 2020, 4, 015004.	4.2	8
588	A charge density prediction model for hydrocarbons using deep neural networks. Machine Learning: Science and Technology, 2020, 1, 025003.	5.0	15
589	Microscopic derivation of density functional theory for superfluid systems based on effective action formalism. Progress of Theoretical and Experimental Physics, 2021, 2021, .	6.6	7
591	Phase change memory materials: Rationalizing the dominance of Ge/Sb/Te alloys. Physical Review B, 2020, 101, .	3.2	22
592	Influence of finite temperature exchange-correlation effects in hydrogen. Physical Review B, 2020, 101,	3.2	44
593	Towards novel organic high- <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:msub><mml:mi>T</mml:mi><mml:mi>c</mml:mi>< superconductors: Data mining using density of states similarity search. Physical Review Materials, 2018, 2, .</mml:msub></mml:math>	/mml:msu 2.4	b _{}{} /mml:ma
594	Vibrational and dielectric properties of the bulk transition metal dichalcogenides. Physical Review Materials, 2018, 2, .	2.4	25
595	Cubic and tetragonal perovskites from the random phase approximation. Physical Review Materials, 2019, 3, .	2.4	10
596	Electron-electron versus electron-phonon interactions in lattice models: Screening effects described by a density functional theory approach. Physical Review Research, 2019, 1, .	3.6	5
597	Effective Hamiltonian for nickelate oxides <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mrow><mml:msub><mml:mi>Nd</mml:mi><mml:mphysical .<="" 2,="" 2020,="" research,="" review="" td=""><td>nr(3w6> < mn</td><td>nl:nsn>1</td></mml:mphysical></mml:msub></mml:mrow></mml:math>	nr (3w6 > < mn	nl :ns n>1
598	Spectral properties of heterostructures containing half-metallic ferromagnets in the presence of local many-body correlations. Physical Review Research, 2020, 2, .	3.6	2
599	First-principles approach with a pseudohybrid density functional for extended Hubbard interactions. Physical Review Research, 2020, 2, .	3.6	31
600	Committee machine that votes for similarity between materials. IUCrJ, 2018, 5, 830-840.	2.2	5
601	Quantifying the effect of interactions in quantum many-body systems. , 0, , .		9
602	Accelerated variational algorithms for digital quantum simulation of many-body ground states. Quantum - the Open Journal for Quantum Science, 0, 4, 324.	0.0	17
603	Basics of the density functional theory. AIMS Materials Science, 2017, 4, 1372-1405.	1.4	13
604	Computational Materials Design. Advances in Chemical and Materials Engineering Book Series, 2016, , 1-12.	0.3	1

#	ARTICLE	IF	CITATIONS
605	Deep-Learning Estimation of Band Gap with the Reading-Periodic-Table Method and Periodic Convolution Layer. Journal of the Physical Society of Japan, 2020, 89, 124006.	1.6	1
606	Assessing cathode property prediction <i>via</i> exchange-correlation functionals with and without long-range dispersion corrections. Physical Chemistry Chemical Physics, 2021, 23, 24726-24737.	2.8	8
607	Experimental studies and DFT calculations to predict atomic arrangements at twin boundaries and distribution behaviors of different solutes in complex intermetallics. Journal of Physics and Chemistry of Solids, 2022, 161, 110453.	4.0	4
608	Testing density functional theory in a quantum Ising chain. Physical Review B, 2021, 104, .	3.2	2
609	Nonlocal exchange and correlation energy functionals using the Yukawa potential as ingredient: Application to the linear response of the uniform electron gas. Physical Review B, 2021, 104, .	3.2	0
610	Fermi Surface Modeling of Lightâ€Rareâ€Earth Hexaborides using Positron Annihilation Spectroscopy. Physica Status Solidi (B): Basic Research, 2022, 259, 2100151.	1.5	0
611	Full Assignment of Ab-Initio Raman Spectra at Finite Temperatures Using Wannier Polarizabilities: Application to Cyclohexane Molecule in Gas Phase. Micromachines, 2021, 12, 1212.	2.9	2
612	Metallic Hydrogen: A Liquid Superconductor?. Journal of Physical Chemistry C, 2021, 125, 23349-23355.	3.1	0
613	Tempering stochastic density functional theory. Journal of Chemical Physics, 2021, 155, 204105.	3.0	3
614	Decoupling thermoelectric transport coefficients of Dirac semimetal Na2AgSb with intrinsically ultralow lattice thermal conductivity. Materials Today Physics, 2021, 21, 100560.	6.0	5
615	Fluid descriptions of quantum plasmas. Reviews of Modern Plasma Physics, 2021, 5, 1.	4.1	16
616	Bead-milling and recrystallization from natural marmatite to Fe-doping ZnS-C materials for lithium-ion battery anodes. Electrochimica Acta, 2021, 399, 139430.	5.2	12
617	A theoretical screening of the O Hâ‹â‹â‹ï€ interaction between water and benzene using density-functional approaches: Effects of nonlocal exchange and long-range dispersion corrections in the true minimum. Computational and Theoretical Chemistry, 2021, 1206, 113464.	2.5	5
618	Harnessing aromaticity to obtain new powerful organic superbases based on phosphaallene ylide scaffold: A density functional theory study. Computational and Theoretical Chemistry, 2021, 1206, 113469.	2.5	4
619	Conventional Approaches to Materials Design. , 2016, , 13-24.		0
620	Iron Oxides Applied to Catalysis. , 2017, , 409-425.		2
621	First-principles calculations of antimony sulphide Sb2S3. Malaysian Journal of Fundamental and Applied Sciences, 2017, 13, .	0.8	4
622	Recent Advances in the Theory of Non-carbon Nanotubes. , 2018, , 352-391.		1

#	Article	IF	CITATIONS
623	Importance of Atomic-Like Basis Set Optimization for DFT Modelling of Nanomaterials. Bulletin of the South Ural State University Series Mathematics Mechanics Physics, 2019, 11, 44-50.	0.2	1
625	Computational Prediction of Estrogenic Micropollutants Removal from Lignin Surface Using Ionic Liquids. Journal of Applied Biotechnology Reports, 2019, 6, 125-128.	0.9	0
626	Density Functional Theory for Magnetism and Magnetic Anisotropy. , 2020, , 895-917.		0
627	Density Functional Theory Calculations Applied to Nuclear Fuels. , 2020, , 2121-2140.		0
628	Electron and Phonon Transport. Mechanical Engineering Series, 2020, , 255-343.	0.2	0
629	Theoretical Insights About the Chemical Dependent Role of Exchange-Correlation Functionals: A Case Study. Engineering Materials, 2020, , 341-357.	0.6	1
630	Computational Auxiliary for the Progress of Sodium-Ion Solid-State Electrolytes. ACS Nano, 2021, 15, 17232-17246.	14.6	42
631	B-F bonding and reactivity analysis of mono- and perfluoro-substituted derivatives of closo-borate anions (6, 10, 12): A computational study. Polyhedron, 2022, 211, 115559.	2.2	8
632	Machine-learning adsorption on binary alloy surfaces for catalyst screening. Chinese Journal of Chemical Physics, 2020, 33, 703-711.	1.3	9
633	Possibility of metastable atomic metallic hydrogen. Physical Review B, 2020, 102, .	3.2	6
634	Robust All-Electron Optimization in Orbital-Free Density-Functional Theory Using the Trust-Region Image Method. Journal of Physical Chemistry A, 2021, 125, 459-475.	2.5	8
635	From Li clusters to nanocatalysis: A brief tour of 40Âyears of cluster chemistry. Inorganica Chimica Acta, 2022, 530, 120680.	2.4	1
636	Theoretical Methods. SpringerBriefs in Applied Sciences and Technology, 2020, , 19-24.	0.4	0
638	Machine learning the derivative discontinuity of density-functional theory. Machine Learning: Science and Technology, 2022, 3, 015011.	5.0	10
639	Pt-Free Metal Nanocatalysts for the Oxygen Reduction Reaction Combining Experiment and Theory: An Overview. Molecules, 2021, 26, 6689.	3.8	11
640	<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mi>L</mml:mi></mml:math> -hole pockets of the Fermi surface of palladium revealed by positron annihilation spectroscopy. Physical Review B, 2021, 104, .	3.2	1
641	Few-fs resolution of a photoactive protein traversing a conical intersection. Nature, 2021, 599, 697-701.	27.8	33
642	Evidence for †Unusual†Exchange†Correlation on Si(111) 7x7: Limitations of Density Functional Calculations for Charge Transfer Interactions on Semiconductor Surfaces Physica Status Solidi (B): Basic Research, 0, , 2100232.	1.5	1

#	Article	IF	CITATIONS
643	Elevating density functional theory to chemical accuracy for water simulations through a density-corrected many-body formalism. Nature Communications, 2021, 12, 6359.	12.8	45
644	Investigating the Electronic Properties of a Composite Dielectric under an Applied Electric Field by Muon Spectroscopy. , 2020, , .		0
645	Computics Approach toward Clarification of Atomic Reactions during Epitaxial Growth of GaN. , 2020, , .		1
646	Hg adatoms on graphene: A first-principles study. JPhys Materials, 2020, 4, 015002.	4.2	0
647	Phase Diagram of Electron–Hole Liquid in Monolayer Heterostructures Based on Transition Metal Dichalcogenides. Journal of Experimental and Theoretical Physics, 2021, 133, 494-507.	0.9	3
648	Scaling analysis of a physics-guided kinetic energy density expansion. Journal of Physics: Conference Series, 2021, 2090, 012123.	0.4	O
649	Role of Defect Engineering and Surface Functionalization in the Design of Carbon Nanotube-Based Nitrogen Oxide Sensors. International Journal of Molecular Sciences, 2021, 22, 12968.	4.1	10
650	Momentum distribution of the uniform electron gas at finite temperature: Effects of spin polarization. Physical Review E, 2021, 104, 055206.	2.1	10
651	Electronic correlations and Fermi liquid behavior of intermediate-band states in titanium-doped silicon. Physical Review B, 2021, 104, .	3.2	1
652	Computational approach in lignin structural models: Influence of non-covalent intramolecular interactions on \hat{l}^2O4 bond properties. Journal of Molecular Structure, 2022, 1251, 131938.	3.6	5
653	Unity of Kohn-Sham density-functional theory and reduced-density-matrix-functional theory. Physical Review A, 2021, 104, .	2.5	11
654	Dzyaloshinskii-Moriya anisotropy effect on field-induced magnon condensation in the kagome antiferromagnet <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mrow><mml:mi>α</mml:mi><mml:mtext>â^'<td>l:mtext><</td><td>mml:msub></td></mml:mtext></mml:mrow></mml:math>	l:mtext><	mml:msub>
655	Computational modeling of green hydrogen generation from photocatalytic H2S splitting: Overview and perspectives. Journal of Photochemistry and Photobiology C: Photochemistry Reviews, 2021, 49, 100456.	11.6	15
656	Molecular Bonding in an Orbital-Free-Related Density Functional Theory. Journal of Physical Chemistry A, 2022, 126, 325-332.	2.5	5
657	Impact ionization and multiple photon absorption in the two-dimensional photoexcited Hubbard model. Physical Review B, 2022, 105 , .	3.2	4
658	Polarizability in Astrochemical Studies of Complex Carbon-Based Compounds. ACS Earth and Space Chemistry, 2022, 6, 1-17.	2.7	7
660	Density-functional theory of material design: fundamentals and applications-I. Oxford Open Materials Science, 2020, 1, .	1.8	2
662	A Submatrix-Based Method for Approximate Matrix Function Evaluation in the Quantum Chemistry Code CP2K., 2020,,.		2

#	Article	IF	CITATIONS
663	Autoencoder-aided analysis of low-dimensional Hilbert spaces. Lithuanian Journal of Physics, 2021, 61, .	0.4	0
664	Portable Acceleration of Materials Modeling Software: CASTEP, GPUs, and OpenACC. Computing in Science and Engineering, 2022, 24, 46-55.	1.2	4
665	Density-Corrected DFT Explained: Questions and Answers. Journal of Chemical Theory and Computation, 2022, 18, 817-827.	5.3	33
666	Site Density Functional Theory and Structural Bioinformatics Analysis of the SARS-CoV Spike Protein and hACE2 Complex. Molecules, 2022, 27, 799.	3.8	5
667	Huzinaga projection embedding for efficient and accurate energies of systems with localized spin-densities. Journal of Chemical Physics, 2022, 156, 054112.	3.0	5
668	gpaw-tools – higher-level user interaction scripts for GPAW calculations and interatomic potential based structure optimization. Computational Materials Science, 2022, 204, 111201.	3.0	3
669	Deep transfer learning correlation study of electronic and spin properties in buckled III-V monolayers. Physica E: Low-Dimensional Systems and Nanostructures, 2022, 140, 115130.	2.7	1
670	Nonlinear interaction of external perturbations in warm dense matter. Contributions To Plasma Physics, 0, , .	1.1	6
671	Improving Density Functional Prediction of Molecular Thermochemical Properties with a Machine-Learning-Corrected Generalized Gradient Approximation. Journal of Physical Chemistry A, 2022, 126, 970-978.	2.5	4
672	Methane conversion into C2 hydrocarbons promoted by N2 over MoP (001) surface: A DFT investigation. Materials Chemistry and Physics, 2022, 281, 125800.	4.0	3
673	Thermal Energy Transport in Oxide Nuclear Fuel. Chemical Reviews, 2022, 122, 3711-3762.	47.7	37
674	A Comparison of Exact and Model Exchange–Correlation Potentials for Molecules. Journal of Physical Chemistry Letters, 2021, 12, 12012-12019.	4.6	13
675	Evaluating the effectiveness of <i>in situ</i> characterization techniques in overcoming mechanistic limitations in lithium–sulfur batteries. Energy and Environmental Science, 2022, 15, 1423-1460.	30.8	37
676	Characterization of Pertechnetates Atco4: A First-Principles Study. SSRN Electronic Journal, 0, , .	0.4	0
677	The duhka of DFT: a noble path to better functionals via a point electron approximation for the exchange $\hat{a} \in \mathbb{C}$. Australian Journal of Chemistry, 2022, , .	0.9	2
678	X-Ray Induced Coloration Behavior of Lu2o3:Eu Transparent Ceramics and the Impact of Zro2 and Hfo2 Sintering Additives. SSRN Electronic Journal, 0, , .	0.4	0
679	From six to eight Î-electron bare rings of group-XIV elements and beyond: can planarity be deciphered from the "quasi-molecules―they embed?. Physical Chemistry Chemical Physics, 2022, 24, 8488-8507.	2.8	5
680	Assessment of Various Density Functional Theory Methods for Finding Accurate Structures of Actinide Complexes. Molecules, 2022, 27, 1500.	3.8	2

#	Article	IF	CITATIONS
681	Pathologies related to abnormal deposits in dermatology: a physico-chemical approach. Comptes Rendus Chimie, 2022, 25, 445-476.	0.5	10
682	Functional-Based Description of Electronic Dynamic and Strong Correlation: Old Issues and New Insights. Journal of Physical Chemistry Letters, 2022, 13, 1744-1751.	4.6	6
683	Power functional theory for many-body dynamics. Reviews of Modern Physics, 2022, 94, .	45.6	31
684	Single Excitation Energies Obtained from the Ensemble "HOMO–LUMO Gap†Exact Results and Approximations. Journal of Physical Chemistry Letters, 2022, 13, 2452-2458.	4.6	14
685	Systematic Improvability in Quantum Embedding for Real Materials. Physical Review X, 2022, 12, .	8.9	14
686	The Nexus between ASAT and Density Functional Theory. , 2022, , 201-221.		0
687	Phase stability of the argon crystal: first-principles study based on random phase approximation plus renormalized single excitation corrections. New Journal of Physics, 2022, 24, 033049.	2.9	4
688	Density functional simulations of a conductive bridging random access memory cell: Ag filament formation in amorphous <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:msub><mml:mi>GeS</mml:mi><mml:mn>2<td>mn^{2,4}/mm</td><td>l:msub></td></mml:mn></mml:msub></mml:math>	mn ^{2,4} /mm	l:msub>
689	<pre><mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mrow><mml:mi>DFT</mml:mi><mml:mo>+î£<mml:mn>2</mml:mn></mml:mo></mml:mrow></mml:math> method for electron correlation effects at transition metal surfaces. Physical Review B, 2022, 105, .</pre>	mo>∢mml 3. <u>2</u>	:mşub> <mml< td=""></mml<>
690	Prediction of Maximum Absorption Wavelength Using Deep Neural Networks. Journal of Chemical Information and Modeling, 2022, 62, 1368-1375.	5.4	12
691	Simulating the Electronic Structure of Spin Defects on Quantum Computers. PRX Quantum, 2022, 3, .	9.2	18
692	Hubbard-corrected oxide formation enthalpies without adjustable parameters. Journal of Physics Communications, 2022, 6, 035009.	1.2	5
694	Accelerating the Convergence of Self-Consistent Field Calculations Using the Many-Body Expansion. Journal of Chemical Theory and Computation, 2022, 18, 179-191.	5.3	6
695	Reply to the "Comment on â€~Experimental Evidence for a New Two-Dimensional Honeycomb Phase of Silicon: A Missing Link in the Chemistry and Physics of Silicon Surfaces?'― Journal of Physical Chemistry C, 2022, 126, 868-869.	3.1	0
696	A DFT+U look into experimentally synthesized monoclinic scheelite BiVO ₄ . Journal of Applied Physics, 2021, 130, 235107.	2.5	7
697	X-ray diffraction and Density Functional Theory based structural analyses of 2-phenyl-4-(prop-2-yn-1-yl)-1,2,4-triazolone. European Journal of Chemistry, 2021, 12, 459-468.	0.6	0
698	It's Complicated: On Relativistic Effects and Periodic Trends in the Melting and Boiling Points of the Group 11 Coinage Metals. Journal of the American Chemical Society, 2022, 144, 485-494.	13.7	6
699	Artificial intelligence-enhanced quantum chemical method with broad applicability. Nature Communications, 2021, 12, 7022.	12.8	52

#	ARTICLE	IF	CITATIONS
700	Understanding Battery Interfaces by Combined Characterization and Simulation Approaches: Challenges and Perspectives. Advanced Energy Materials, 2022, 12, .	19.5	46
701	Single-momentum path integral Monte Carlo simulations of uniform electron gas in warm dense matter regime. Physics of Plasmas, 2021, 28, 122712.	1.9	1
702	An Entropic Approach to Classical Density Functional Theory. , 2021, 3, .		0
703	Reformulation of thermally assisted-occupation density functional theory in the Kohn–Sham framework. Journal of Chemical Physics, 2022, 156, 174108.	3.0	6
704	Numerical quality control for DFT-based materials databases. Npj Computational Materials, 2022, 8, .	8.7	6
705	Nanostructured materials and heterogeneous catalysis: a succinct review regarding DeNox catalysis. Comptes Rendus Chimie, 2022, 25, 237-244.	0.5	5
707	The Uniform Electron Gas at High Temperatures: Ab Initio Path Integral Monte Carlo Simulations and Analytical Theory. SSRN Electronic Journal, 0, , .	0.4	0
708	Machine learning-based prediction of the adsorption energy for CO on boron-doped graphene. New Journal of Chemistry, 0, , .	2.8	1
709	Quantum surface effects in the electromagnetic coupling between a quantum emitter and a plasmonic nanoantenna: time-dependent density functional theory vs. semiclassical Feibelman approach. Optics Express, 2022, 30, 21159.	3.4	7
710	Convert Widespread Paraelectric Perovskite to Ferroelectrics. Physical Review Letters, 2022, 128, .	7.8	5
711	Lattice dynamical properties of antiferromagnetic oxides calculated using self-consistent extended Hubbard functional method. Journal of Physics Condensed Matter, 2022, , .	1.8	2
712	2D MBenes: A Novel Member in the Flatland. Advanced Materials, 2022, 34, e2108840.	21.0	54
713	Connector theory for reusing model results to determine materials properties. Npj Computational Materials, 2022, 8, .	8.7	2
714	Linear-time generalized Hartree-Fock algorithm for quasi-one-dimensional systems. Physical Review Research, 2022, 4, .	3.6	1
715	xmlns:mml="http://www.w3.org/1998/Math/MathML"> <mml:mrow><mml:mi>A</mml:mi><mml:mi>b</mml:mi> <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mrow><mml:mi>i</mml:mi><mml:mi>n</mml:mi>< point defect calculations for structural properties of a model austenitic steel alloy. Physical Review</mml:mrow></mml:math></mml:mrow>		
716	Materials, 2022, 6, . Reducing the internal reorganization energy ⟨i⟩via⟨/i⟩ symmetry controlled Ï€-electron delocalization. Chemical Science, 2022, 13, 7181-7189.	7.4	14
717	$\label{lem:hyberd} Hubbard < mml:math $$xmlns:mml="http://www.w3.org/1998/Math/MathML">< mml:mi>U parameters for transition metals from first principles. Physical Review B, 2022, 105, .$	3.2	23
718	The chemical bond in solidsâ€"revisited. Journal of Physics Condensed Matter, 2022, 34, 343001.	1.8	6

#	Article	IF	CITATIONS
719	Green's Function Formulation of Quantum Defect Embedding Theory. Journal of Chemical Theory and Computation, 2022, 18, 3512-3522.	5.3	17
720	Optimization of the r ² SCAN-3c Composite Electronic-Structure Method for Use with Slater-Type Orbital Basis Sets. Journal of Physical Chemistry A, 2022, 126, 3826-3838.	2.5	8
721	Efficient Integral-Direct Methods for Self-Consistent Reduced Density Matrix Functional Theory Calculations on Central and Graphics Processing Units. Journal of Chemical Theory and Computation, 2022, 18, 4229-4244.	5.3	6
722	Computational methods to simulate molten salt thermophysical properties. Communications Chemistry, 2022, 5, .	4.5	17
723	Study to amino acid-based inhibitors as an effective anti-corrosion material. Journal of Molecular Liquids, 2022, 360, 119449.	4.9	7
725	Deep-learning density functional theory Hamiltonian for efficient ab initio electronic-structure calculation. Nature Computational Science, 2022, 2, 367-377.	8.0	38
726	DFTB Parameters for the Periodic Table: Part III, Spin-Orbit Coupling. Journal of Chemical Theory and Computation, 0, , .	5.3	5
727	Improving the efficiency of ab initio electronic-structure calculations by deep learning. Nature Computational Science, 2022, 2, 418-419.	8.0	3
728	Solid-state performance of a meta-GGA screened hybrid density functional constructed from Pauli kinetic enhancement factor dependent semilocal exchange hole. Journal of Chemical Physics, 0, , .	3.0	4
729	Assessing the accuracy of compound formation energies with quantum Monte Carlo. Physical Review B, 2022, 105 , .	3.2	2
730	Study the application of new type green corrosion inhibitors for iron metal. Inorganic Chemistry Communication, 2022, 142, 109650.	3.9	6
731	X-ray induced coloration behavior of Lu2O3:Eu transparent ceramics and the impact of ZrO2 and HfO2 sintering additives. Optical Materials, 2022, 131, 112641.	3.6	4
733	Momentum Distribution Functions and Pair Correlation Functions of Unpolarized Uniform Electron Gas in Warm Dense Matter Regime. Mathematics, 2022, 10, 2270.	2.2	1
734	Materials challenges for successful roll-out of commercial fusion reactors. JPhys Energy, 2022, 4, 030401.	5.3	0
735	Machine Learning Modeling for Accelerated Battery Materials Design in the Small Data Regime. Advanced Energy Materials, 2022, 12, .	19.5	29
736	Spin-resolved density response of the warm dense electron gas. Physical Review Research, 2022, 4, .	3.6	12
737	On modeling the induced charge in density-functional calculations for field emitters. Journal of Vacuum Science and Technology B:Nanotechnology and Microelectronics, 2022, 40, 042802.	1.2	3
738	Designing Rashba systems for high thermoelectric performance based on the van der Waals heterostructure. Materials Today Physics, 2022, 27, 100788.	6.0	1

#	Article	IF	CITATIONS
739	Adsorption of small gas molecules of transition metal (Pt and Au) modified HfSe2 monolayer. Materials Today Communications, 2022, 32, 103885.	1.9	0
740	Identifying Redox Orbitals and Defects in Lithium-Ion Cathodes with Compton Scattering and Positron Annihilation Spectroscopies: A Review. Condensed Matter, 2022, 7, 47.	1.8	3
741	Quantum embedding theories to simulate condensed systems on quantum computers. Nature Computational Science, 2022, 2, 424-432.	8.0	19
742	An interpretation of quantum foundations based on density functional theory and polymer self-consistent field theory. Quantum Studies: Mathematics and Foundations, 0, , .	0.9	4
743	Nanomaterials in medicine: a concise review of nanomaterials intended to treat pathology, nanomaterials induced by pathology, and pathology provoked by nanomaterials. Comptes Rendus Chimie, 2022, 25, 165-188.	0.5	3
744	Static Electronic Density Response of Warm Dense Hydrogen: <i>AbÂlnitio</i> Path Integral MonteÂCarlo Simulations. Physical Review Letters, 2022, 129, .	7.8	21
745	Extensibility of Hohenberg–Kohn Theorem to General Quantum Systems. Advanced Quantum Technologies, 2022, 5, .	3.9	2
746	Deriving force fields with a multiscale approach: From <i>ab initio</i> calculations to molecular-based equations of state. Journal of Chemical Physics, 2022, 157, .	3.0	2
747	Constraintâ€based analysis of a physicsâ€guided kinetic energy density expansion. International Journal of Quantum Chemistry, 0, , .	2.0	1
748	DFT simulation of conductivity of the p-type doped and charge-injected cis-polyacetylene. Molecular Physics, 0, , .	1.7	1
749	Correct and Accurate Polymorphic Energy Ordering of Transition-Metal Monoxides Obtained from Semilocal and Onsite-Hybrid Exchange-Correlation Approximations. Journal of Physical Chemistry C, 2022, 126, 14650-14660.	3.1	4
750	Multistate Density Functional Theory of Excited States. Journal of Physical Chemistry Letters, 2022, 13, 7762-7769.	4.6	18
751	Pseudo pair potential between protons in dense hydrogen from first principles. Molecular Physics, 0, ,	1.7	0
752	Interfacial charge transfer and Schottky barriers at c-Si/a-In heterojunctions. Journal of Physics Communications, 2022, 6, 085010.	1.2	0
753	Advances and Challenges in DFT-based Energy Materials Design. Chinese Physics B, 0, , .	1.4	8
754	Changes in polarization dictate necessary approximations for modeling electronic deexcitation intensity: Application to x-ray emission. Physical Review B, 2022, 106, .	3.2	4
755	Large-Scale DFT Methods for Calculations of Materials with Complex Structures. Journal of the Physical Society of Japan, 2022, 91, .	1.6	3
756	A DFT+U approach to doped SrTiO3 for solar harvesting applications. Computational Materials Science, 2022, 214, 111743.	3.0	6

#	Article	IF	CITATIONS
757	Dimethyl fumarate molecule, crystal, and plane: Optical absorption measurement and structural/optoelectronic properties by density functional theory calculations. Journal of Physics and Chemistry of Solids, 2022, 170, 110958.	4.0	0
758	First-principles study of Co21W18 with pressure effect: The structural, mechanical, electronic properties and Debye temperature. Materials Today Communications, 2022, 33, 104276.	1.9	2
759	Self-Consistent Implementation of Kohn–Sham Adiabatic Connection Models with Improved Treatment of the Strong-Interaction Limit. Journal of Chemical Theory and Computation, 2022, 18, 5936-5947.	5. 3	8
760	Characterization of the binding interaction between atrazine and human serum albumin: Fluorescence spectroscopy, molecular dynamics and quantum biochemistry. Chemico-Biological Interactions, 2022, 366, 110130. First-principles study of <mml:math.xmlns:mml="http: 1998="" math="" mathml"<="" td="" www.w3.org=""><td>4.0</td><td>6</td></mml:math.xmlns:mml="http:>	4.0	6
761	altimg="si71.svg" display="inline" id="d1e3448"> <mml:mi>A</mml:mi> TcO <mml:math altimg="si72.svg" display="inline" id="d1e3453" xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:msub><mml:mrow></mml:mrow><mml:mrow></mml:mrow></mml:msub><td>4.0</td><td>4</td></mml:math>	4.0	4
762	of Physics and Chemistry of Solids, 2022, 171, 110979. TTDFT: A GPU accelerated Tucker tensor DFT code for large-scale Kohn-Sham DFT calculations. Computer Physics Communications, 2023, 282, 108516.	7.5	1
763	Density-functional theory., 2023,, 27-65.		0
764	Multi-Fidelity Learning. Synthesis Lectures on Materials and Optics, 2020, , 135-152.	0.2	0
765	Structural diversity of CuZn ₂ InSe ₄ quaternary chalcogenides: electronic and phonon properties from first principles. RSC Advances, 2022, 12, 26648-26656.	3.6	3
766	Density Functional Theory., 2022,, 1-16.		0
767	Dynamical mean-field theory for spin-dependent electron transport in spin-valve devices. Physical Review B, 2022, 106 , .	3.2	4
768	Dynamical triplet unraveling : A quantum Monte Carlo algorithm for reversible dynamics. Physical Review A, 2022, 106, .	2.5	0
769	Efficient enumeration-selection computational strategy for adaptive chemistry. Scientific Reports, 2022, 12, .	3.3	0
770	The usefulness of the first-principles calculations of optical properties of the materials and the type of information that can be accessed by them. Optical Materials: X, 2022, 15, 100185.	0.8	0
771	Efficient and improved prediction of the band offsets at semiconductor heterojunctions from meta-GGA density functionals: A benchmark study. Journal of Chemical Physics, 2022, 157, .	3.0	5
773	Evolving symbolic density functionals. Science Advances, 2022, 8, .	10.3	13
774	Advances in actinide thin films: synthesis, properties, and future directions. Reports on Progress in Physics, 2022, 85, 123101.	20.1	4
775	Electronic Configurations of 3d Transition-Metal Compounds Using Local Structure and Neural Networks. Journal of Physical Chemistry A, 2022, 126, 7373-7381.	2.5	3

#	Article	IF	CITATIONS
776	Effect of Segregation of Sc, Y and La Atoms on Prenucleation at the Liquid-Al/ \hat{I}^3 -Al2O3 $\{1\ 1\ 1\}$ Interfaces. Metals, 2022, 12, 1550.	2.3	2
777	Flipping Kinetics of the Water Trimer on Acenaphthylene: Persistence of a Highly Dipolar <i>ddd</i> Configuration at Interstellar Temperatures. ACS Earth and Space Chemistry, 2022, 6, 2282-2294.	2.7	1
778	Heterointerface effects of lithium intercalation and diffusion in van der Waals heterostructures. Physical Review Materials, 2022, 6, .	2.4	4
779	The mean-field concept and post-DMFT methods in the contemporary theory of correlated systems. Physics-Uspekhi, O, , .	2.2	0
780	Machine learning accelerated DFT research on platinum-modified amorphous alloy surface catalysts. Chinese Chemical Letters, 2023, 34, 107833.	9.0	4
781	On the kinetic energy density functional: the limit of the density derivative order. Physica Scripta, 0, , .	2.5	0
782	How good are recent density functionals for ground and excited states of one-electron systems?. Journal of Chemical Physics, 2022, 157, .	3.0	6
783	Magneto-optical detection of topological contributions to the anomalous Hall effect in a kagome ferromagnet. Physical Review B, 2022, 106, .	3.2	2
784	Theoretical SERS study of the strength and suitability of Cu12 nanostar for SERS: Complete theoretical studies, coinage metal SM12 comparisons, benzothiazole (BTH) adsorbent. Computational and Theoretical Chemistry, 2022, 1217, 113889.	2.5	8
785	Pressure-induced structural phase transitions of zirconium: an ab initio study based on statistical ensemble theory. Journal of Physics Condensed Matter, 2022, 34, 505402.	1.8	1
786	Finite-temperature properties of extended Nagaoka ferromagnetism: Ordering processes and precursor of a quantum phase transition between itinerant ferromagnetic and Mott antiferromagnetic states. Physical Review B, 2022, 106, .	3.2	0
787	Intramolecular Interactions in Derivatives of Uracil Tautomers. Molecules, 2022, 27, 7240.	3.8	2
788	Many recent density functionals are numerically ill-behaved. Journal of Chemical Physics, 2022, 157, .	3.0	14
789	Minimal Active Space: NOSCF and NOSI in Multistate Density Functional Theory. Journal of Chemical Theory and Computation, 2022, 18, 6407-6420.	5.3	8
790	Substructure interaction graph network with node augmentation for hybrid chemical systems of heterogeneous substructures. Computational Materials Science, 2023, 216, 111835.	3.0	1
791	Perspectives on weak interactions in complex materials at different length scales. Physical Chemistry Chemical Physics, 2023, 25, 2671-2705.	2.8	10
792	A comprehensive study of the reduction of nitrate on natural FeTiO3: Photocatalysis and DFT calculations. Separation and Purification Technology, 2023, 306, 122570.	7.9	4
793	Ab initio Methods for Electronic Transport in Semiconductors and Nanostructures. Springer Handbooks, 2023, , 1515-1558.	0.6	0

#	Article	IF	CITATIONS
794	Magnetic hopfions in solids. APL Materials, 2022, 10, .	5.1	27
795	Electronic band gap on graphene induced by interaction with hydrogen cyanide. An DFT analysis. Chemical Physics, 2023, 565, 111744.	1.9	5
796	Pressure-induced ferroelectric transition in LiBC. Physical Review B, 2022, 106, .	3.2	0
797	Ab initio study of RaWO4: Comparison with isoelectronic tungstates. Journal of Solid State Chemistry, 2023, 317, 123709.	2.9	2
798	The uniform electron gas at high temperatures: ab initio path integral Monte Carlo simulations and analytical theory. High Energy Density Physics, 2022, 45, 101015.	1.5	9
799	Models for Pairing Phenomena. , 2022, , 1-34.		0
800	An ab initio study of structural phase transitions of crystalline aluminium under ultrahigh pressures based on ensemble theory. Computational Materials Science, 2023, 218, 111960.	3.0	1
801	A structural optimization algorithm with stochastic forces and stresses. Nature Computational Science, 2022, 2, 736-744.	8.0	4
802	Large Scale Quantum Chemistry with Tensor Processing Units. Journal of Chemical Theory and Computation, 2023, 19, 25-32.	5.3	12
803	Ab initio calculation of real solids via neural network ansatz. Nature Communications, 2022, 13, .	12.8	11
804	Synchrotron-based techniques for characterizing STCH water-splitting materials. Frontiers in Energy Research, $0,10,1$	2.3	1
805	Stability of FeVO4-II under Pressure: A First-Principles Study. Crystals, 2022, 12, 1835.	2.2	4
806	The effects of electron-phonon coupling on the phonon transport properties of the Weyl semimetals NbAs and TaAs: A comparative study. Journal of Materiomics, 2022, , .	5.7	2
807	Spin–orbit coupling corrections for the GFN-xTB method. Journal of Chemical Physics, 2023, 158, .	3.0	3
808	Accuracy of electronic density calculated using an optimally tuned range-separated hybrid functional. Theoretical Chemistry Accounts, 2023, 142 , .	1.4	1
809	Computational Workflow forÂAccelerated Molecular Design Using Quantum Chemical Simulations andÂDeep Learning Models. Communications in Computer and Information Science, 2022, , 3-19.	0.5	1
810	On the role of torsional dynamics in the solid-state fluorescent properties of a new bifluorene–tetracarboxylic acid and its supramolecular assemblies: a structural and TD-DFT investigation. CrystEngComm, 2023, 25, 1058-1066.	2.6	4
811	Local Corrosion Behaviors in the Coarse-Grained Heat-Affected Zone in a Newly Developed Zr–Ti–Al–RE Deoxidized High-Strength Low-Alloy Steel. Materials, 2023, 16, 876.	2.9	0

#	Article	IF	CITATIONS
812	On the Origins of Spontaneous Spherical Symmetry-Breaking in Open-Shell Atoms Through Polymer Self-Consistent Field Theory. Journal of Chemical Physics, 0, , .	3.0	0
813	Density Matrix Implementation of the Fermi–Löwdin Orbital Self-Interaction Correction Method. Journal of Physical Chemistry A, 2023, 127, 527-534.	2.5	2
814	The Predictive Power of Exact Constraints and Appropriate Norms in Density Functional Theory. Annual Review of Physical Chemistry, 2023, 74, 193-218.	10.8	22
816	Simulation of Complex Biomolecular Systems: The Ribosome Challenge. Annual Review of Biophysics, 2023, 52, 361-390.	10.0	2
817	Site Selective Concerted Nucleophilic Aromatic Substitutions of Azoleâ€Ligated Diaryliodonium Salts. Advanced Synthesis and Catalysis, 2023, 365, 535-543.	4.3	4
818	Combined experimental and DFT approach to BiNbO ₄ polymorphs. RSC Advances, 2023, 13, 5576-5589.	3.6	5
819	Time-dependent exchange-correlation hole and potential of the electron gas. Physical Review B, 2023, 107, .	3.2	2
820	Analysis of Bonding by Quantum Chemistry─Resolving Delocalization Stabilization in a Mechanistic Basis and New Hückel Model. Journal of Physical Chemistry A, O, , .	2.5	0
821	Effect of four-phonon scattering on anisotropic thermal transport in bulk hexagonal boron nitride by machine learning interatomic potential. International Journal of Heat and Mass Transfer, 2023, 207, 124011.	4.8	5
822	Small-data-based machine learning interatomic potentials for graphene grain boundaries enabled by structural unit model. Carbon Trends, 2023, 11, 100260.	3.0	1
823	Spin-state gaps and self-interaction-corrected density functional approximations: Octahedral Fe(II) complexes as case study. Journal of Chemical Physics, 2023, 158, .	3.0	7
824	Recent advances of ferromagnetism in traditional antiferromagnetic transition metal oxides. Journal of Magnetism and Magnetic Materials, 2023, 569, 170428.	2.3	1
825	Ab Initio Static Exchange–Correlation Kernel across Jacob's Ladder without Functional Derivatives. Journal of Chemical Theory and Computation, 2023, 19, 1286-1299.	5.3	14
826	pyGWBSE: a high throughput workflow package for GW-BSE calculations. Npj Computational Materials, 2023, 9, .	8.7	6
827	Synthesis of Disubstituted Carboxonium Derivatives of Closo-Decaborate Anion [2,6-B10H8O2CC6H5]â^: Theoretical and Experimental Study. Molecules, 2023, 28, 1757.	3.8	1
828	Machine learning-aided Genetic algorithm in investigating the structure–property relationship of SmFe12-based structures. Journal of Applied Physics, 2023, 133, .	2.5	2
829	Chemical interactions that govern the structures of metals. Proceedings of the National Academy of Sciences of the United States of America, 2023, 120, .	7.1	2
830	Improving the performance of fermionic neural networks with the <scp>Slater</scp> exponential <i>Ansatz</i> . International Journal of Quantum Chemistry, 0, , .	2.0	0

#	Article	IF	CITATIONS
831	Copula approach to exchange-correlation hole in many-electron systems with strong correlations. Chinese Journal of Chemical Physics, 2023, 36, 685-690.	1.3	0
832	Entangled origins of the nonmagnetic states of U and Fe atoms in hydrogenated UFeGe. Physical Review Materials, 2023, 7, .	2.4	2
833	Restricted multicanonical sampling for machine learning potential construction. Physical Review B, 2023, 107, .	3.2	1
834	Recent advances in density functional theory approach for optoelectronics properties of graphene. Heliyon, 2023, 9, e14279.	3.2	2
835	First Principles Modeling of Strain Induced Effects in Functional Materials. , 2023, , 1-30.		0
836	Electronic density response of warm dense matter. Physics of Plasmas, 2023, 30, .	1.9	23
837	Correlation energy of the paramagnetic electron gas at the thermodynamic limit. Physical Review B, 2023, 107, .	3.2	3
838	Higher-order Rayleigh-quotient gradient effect on electron correlations. Journal of Chemical Physics, 2023, 158, .	3.0	2
839	Simulation of Hafnium-Based FinFET and Ferroelectricity of Related 2-Dimensional Hafnium-Based Materials., 0, 29, 69-76.		0
840	Efficient determination of the Hamiltonian and electronic properties using graph neural network with complete local coordinates. Machine Learning: Science and Technology, 2023, 4, 035010.	5.0	1
841	Competition between phonon-vacancy and four-phonon scattering in cubic boron arsenide by machine learning interatomic potential. Physical Review Materials, 2023, 7, .	2.4	2
842	Quantum version of the integral equation theory-based dielectric scheme for strongly coupled electron liquids. Journal of Chemical Physics, 2023, 158, .	3.0	7
843	Machine learning and DFT investigation of CO, CO ₂ and CH ₄ adsorption on pristine and defective two-dimensional magnesene. Physical Chemistry Chemical Physics, 2023, 25, 13170-13182.	2.8	3
844	A semilocal machine-learning correction to density functional approximations. Journal of Chemical Physics, 2023, 158, .	3.0	1
845	Ab Initio Molecular Dynamics: A Guide to Applications. , 2024, , 493-517.		0
846	Crystal binding (interatomic forces): Metallic bonding and crystals. , 2024, , 217-230.		0
847	Dynamical Stability and Physical Properties of Fe Dihalide Nanowires. Advanced Theory and Simulations, 0 , 0 .	2.8	0
848	Pico technology – An advancement in dye degradation. AIP Conference Proceedings, 2023, , .	0.4	0

#	Article	IF	CITATIONS
849	Towards the construction of an accurate kinetic energy density functional and its functional derivative through physics-informed neural networks. Journal of Physics Communications, 2023, 7, 061001.	1.2	1
850	Electron density to analyze acids and bases of Lewis: computational tools. , 2023, , 313-333.		0
851	Unravelling the adsorption and electroreduction performance of CO ₂ and N ₂ over defective and B, P, Si-doped C ₃ Ns: a DFT study. Physical Chemistry Chemical Physics, 2023, 25, 16952-16961.	2.8	1
852	Carbon-[<i>n</i>]Triangulenes and Sila-[<i>n</i>]Triangulenes: Which Are Planar?. Journal of Physical Chemistry A, 2023, 127, 5048-5064.	2.5	2
853	Materials cartography: A forward-looking perspective on materials representation and devising better maps. , 2023, $1,\ldots$		1
854	Random and block architectures of $\langle i \rangle N \langle i \rangle$ -arylitaconimide monomers with methyl methacrylate. ChemistrySelect, 2023, . Electronic interaction $\langle mm :math$	1.5	0
855	xmlns:mml="http://www.w3.org/1998/Math/MathML"> <mml:msub><mml:mi>U</mml:mi><mml:mrow><mml:mi <mml:math="" on="" oxygen="" xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mi>p</mml:mi> orbitals in oxides: Role of correlated orbitals on the example of <mml:math< td=""><td>>p3.2</td><td>mi><mml:mi></mml:mi></td></mml:math<></mml:mi></mml:mrow></mml:msub>	>p3.2	mi> <mml:mi></mml:mi>
856	xmlns:mml="http://www.w3.org/1998/Math/MathML"> <mml:msub><mml:mi>UO</mml:mi><mml:mn>2<td>nn>2.8</td><td>:msub> 1</td></mml:mn></mml:msub>	nn>2.8	:msub> 1
857	Momentum matching and band-alignment type in van der Waals heterostructures: Interfacial effects and materials screening. Physical Review B, 2023, 107, .	3.2	3
858	MP2-Based Correction Scheme to Approach the Limit of a Complete Pair Natural Orbitals Space in DLPNO-CCSD(T) Calculations. Journal of Chemical Theory and Computation, 0, , .	5. 3	2
859	Efficient Screening of Metal Promoters of Pt Catalysts for C–H Bond Activation in Propane Dehydrogenation from a Combined First-Principles Calculations and Machine-Learning Study. ACS Omega, 0, , .	3.5	0
860	Energy response and spatial alignment of the perturbed electron gas. Journal of Chemical Physics, 2023, 158, .	3.0	2
861	Extraction of the frequency moments of spectral densities from imaginary-time correlation function data. Physical Review B, 2023, 107, .	3.2	5
862	Inhibitory behavior and adsorption of asparagine dipeptide amino acid on the Fe(111) surface. Journal of Molecular Modeling, 2023, 29, .	1.8	1
863	An <i>ab initio</i> DFT perspective on experimentally synthesized CuBi ₂ O ₄ . RSC Advances, 2023, 13, 14291-14305.	3.6	3
864	Effect of surface functional groups on MXene conductivity. Journal of Chemical Physics, 2023, 158, .	3.0	2
865	Computation of forces and stresses in solids: Towards accurate structural optimization with auxiliary-field quantum Monte Carlo. Physical Review B, 2023, 107, .	3.2	4
866	Recent Progress of Amorphous Nanomaterials. Chemical Reviews, 2023, 123, 8859-8941.	47.7	29

#	Article	IF	CITATIONS
867	Predicting electronic structures at any length scale with machine learning. Npj Computational Materials, 2023, 9, interfacial electric field generated during simultaneous HER and OER over Li	8.7	10
868	intercalated <mml:math altimg="si149.svg" display="inline" id="d1e189" xmlns:mml="http://www.w3.org/1998/Math/Math/Math/ME"><mml:mrow><mml:mi>g</mml:mi><mml:mo linebreak="goodbreak" linebreakstyle="after">â^2</mml:mo><mml:msub><mml:mrow><mml:mi mathvariant="normal">C</mml:mi></mml:mrow><mml:mrow><mml:mrow><mml:mn>3</mml:mn></mml:mrow><td>3.0 >><mml:m< td=""><td>o sub><mmlar< td=""></mmlar<></td></mml:m<></td></mml:mrow></mml:msub></mml:mrow></mml:math>	3.0 >> <mml:m< td=""><td>o sub><mmlar< td=""></mmlar<></td></mml:m<>	o sub> <mmlar< td=""></mmlar<>
869	Investigation of Tungstenâ€Based Selenoâ€Chevrel Compounds with Different Compositions for Efficient Water Splitting. Advanced Theory and Simulations, 2023, 6, .	2.8	0
870	Surface metal ion doped TiO2 nanowire arrays by low energy ion implantation for enhanced photoelectrochemical performance. Ceramics International, 2023, , .	4.8	O
871	Simple and effective screening parameter for range-separated dielectric-dependent hybrids. Physical Review B, 2023, 108, .	3.2	2
872	Toward first-principles approaches for mechanistic study of self-trapped exciton luminescence. Chemical Physics Reviews, 2023, 4, .	5.7	2
873	Ab initio quantum chemistry with neural-network wavefunctions. Nature Reviews Chemistry, 2023, 7, 692-709.	30.2	8
874	Physical insights from imaginary-time density–density correlation functions. Matter and Radiation at Extremes, 2023, 8, .	3.9	9
875	Sommerfeld expansion of electronic entropy in an inferno-like average atom model. Physical Review B, 2023, 108, .	3.2	0
876	Neural network interatomic potential for laser-excited materials. Communications Materials, 2023, 4, . The effect of pressure on the band-gap energy in FePO <mml:math< td=""><td>6.9</td><td>2</td></mml:math<>	6.9	2
877	xmlns:mml="http://www.w3.org/1998/Math/MathML" altimg="si60.svg" display="inline" id="d1e774"> <mml:msub><mml:mrow></mml:mrow><mml:mrow></mml:mrow></mml:msub> and FeVO <mml:math <="" altimg="si60.svg" display="inline" td="" xmlns:mml="http://www.w3.org/1998/Math/MathML"><td>4.0</td><td>1</td></mml:math>	4.0	1
878	id="d1e782"> <mml:msub><mml:mrow /><mml:msub></mml:msub></mml:mrow </mml:msub>	3.0	2
879	Tuning electrocatalytic nitrogen reduction on supported nickel cluster via substrate phase engineering. Applied Surface Science, 2023, 640, 158277.	6.1	2
880	Density functional descriptions of interfacial electronic structure. Chemical Physics Reviews, 2023, 4,	5.7	0
881	Identifying Rashba–Dresselhaus splittings from first-principle calculations: A brief overview. Modern Physics Letters B, 2024, 38, .	1.9	1
882	Discovering targeted inhibitors for <i>Escherichia coli</i> efflux pump fusion proteins using computational and structureâ€guided approaches. Journal of Computational Chemistry, 0, , .	3.3	1
883	Homogeneous electron liquid in arbitrary dimensions beyond the random phase approximation. New Journal of Physics, 2023, 25, 083040.	2.9	1
884	Density functional applications of jellium with a local gap model correlation energy functional. Journal of Chemical Physics, 2023, 159, .	3.0	1

#	Article	IF	CITATIONS
885	Reproducibility of density functional approximations: How new functionals should be reported. Journal of Chemical Physics, $2023,159,.$	3.0	1
886	Electronic and Thermal Properties of the Cation Substitution-Derived Quaternary Chalcogenide CulnSnSe ₄ . Inorganic Chemistry, 2023, 62, 16114-16121.	4.0	0
887	Exploring the crystal structure and properties of ytterbium orthoantimonate under high pressure. Dalton Transactions, 2023, 52, 14517-14526.	3.3	1
888	Novel enzymatic tools for C–C bond formation through the development of new-to-nature biocatalysis. Advances in Catalysis, 2023, , .	0.2	0
889	Radiation Defect Formation in a Silicon Carbide Betaconverter. Physics of Particles and Nuclei Letters, 2023, 20, 1094-1097.	0.4	0
890	Tiling a molecule: Is partially hydrogenated graphene planar infinite benzene?. Chemical Physics Letters, 2023, 831, 140836.	2.6	1
891	<tt>koopmans</tt> : An Open-Source Package for Accurately and Efficiently Predicting Spectral Properties with Koopmans Functionals. Journal of Chemical Theory and Computation, 2023, 19, 7097-7111.	5.3	4
892	Models for Pairing Phenomena. , 2023, , 2011-2044.		0
893	Continuity equationÂfor the many-electron spectral function. Physical Review B, 2023, 108, .	3.2	0
894	Revealing the real structure of M7C3 by high-throughput DFT calculations. Computational Materials Science, 2023, 230, 112494.	3.0	1
895	Correlation energy of the spin-polarized electron liquid studied using quantum Monte Carlo simulations. Physical Review B, 2023, 108, .	3.2	0
896	Two-Dimensional Metal–Organic Framework TM Catalysts for Electrocatalytic N2 and CO2 Reduction: A Density Functional Theory Investigation. Crystals, 2023, 13, 1426.	2.2	0
897	Machine learning the electronic structure of matter across temperatures. Physical Review B, 2023, 108, .	3.2	0
898	Polarization Properties of Wurtzite III-Nitride Alloys Using the Hexagonal Reference Structure. ECS Journal of Solid State Science and Technology, 2023, 12, 103008.	1.8	0
899	Cation substitution varieties of I-II2-III-VI4 semiconductors and their effects on electronic and phononic properties. Journal of Alloys and Compounds, 2023, 969, 172399.	5.5	0
900	Density Functional Theory Calculations on the Interstellar Formation of Biomolecules. Research in Astronomy and Astrophysics, 0, , .	1.7	0
901	Opening the Density Functional Theory Black Box: A Collection of Pedagogic Jupyter Notebooks. Journal of Chemical Education, 2023, 100, 4496-4503.	2.3	0
902	Artificial Neural Network-Based Density Functional Approach for Adiabatic Energy Differences in Transition Metal Complexes. Journal of Chemical Theory and Computation, 2023, 19, 7555-7566.	5.3	1

#	Article	IF	CITATIONS
903	Orbital-Free Density Functional Theory: An Attractive Electronic Structure Method for Large-Scale First-Principles Simulations. Chemical Reviews, 2023, 123, 12039-12104.	47.7	7
904	Recent Advancements in Mechanistic Studies of Palladium- and Nickel-Catalyzed Ethylene Copolymerization with Polar Monomers. Polymers, 2023, 15, 4343.	4.5	1
905	Development of a novel hypochlorite ratio probe based on coumarin and its application in living cells. RSC Advances, 2023, 13, 32518-32522.	3.6	0
906	Short-range screened density matrix functional for proper descriptions of thermochemistry, thermochemical kinetics, nonbonded interactions, and singlet diradicals. Journal of Chemical Physics, 2023, 159, .	3.0	0
907	Harness the power of atomistic modeling and deep learning in biofuel separation. Annual Reports in Computational Chemistry, 2023, , 121-165.	1.7	0
908	Multipole Expansion of Atomic Electron Density Fluctuation Interactions in the Density-Functional Tight-Binding Method. Journal of Chemical Theory and Computation, 2023, 19, 7592-7605.	5.3	1
909	Electronic structure and optical properties of superconducting compounds ScGa ₃ and LuGa ₃ . Modern Physics Letters B, O, , .	1.9	0
910	Fermionic physics from <i>abÂinitio </i> path integral Monte Carlo simulations of fictitious identical particles. Journal of Chemical Physics, 2023, 159, .	3.0	2
911	Site occupancy and electronic properties of NbCo2 Laves phases doped with Re. Computational and Theoretical Chemistry, 2023, 1230, 114389.	2.5	0
912	The energy landscape of the ribosome. Biopolymers, 0, , .	2.4	0
913	Leveraging Flavonoids as Potential Inhibitors of METTL3 in Combating Cancer: A Combined Structureâ∈Based Drug Design and DFT Approach. ChemistrySelect, 2023, 8, .	1.5	0
914	Range-Separated Local Hybrid Functionals with Small Fractional-Charge and Fractional-Spin Errors: Escaping the Zero-Sum Game of DFT Functionals. Journal of Chemical Theory and Computation, 2023, 19, 8639-8653.	5.3	2
915	An efficient finite difference approach to solutions of SchrĶdinger equations of atoms in non-linear coordinates. Physica Scripta, 2023, 98, 125409.	2.5	1
916	Enhancing the electrical transport properties of two-dimensional semiconductors through interlayer interactions. Energy and Environmental Science, 0, , .	30.8	0
917	Role of Defects, Impurities and Deviations from the Stoichiometry in the Optoelectronic Properties of Semiconductors., 2023,, 75-141.		0
918	Modeling and Simulation of Nano-devices. , 2024, , 1881-1891.		0
920	A combined first principles and experimental approach to Bi ₂ WO ₆ . RSC Advances, 2023, 13, 36130-36143.	3.6	2
921	Exploring the potential of porphyrin-based materials for organic solar cells supported on carbon: A quantum chemistry approach. Journal of Photochemistry and Photobiology A: Chemistry, 2024, 449, 115401.	3.9	0

#	Article	IF	CITATIONS
922	Quantifying errors of electron-proton/muon correlation functionals through the Kohn-Sham inversion of a two-component model system. Physical Review B, 2023, 108, .	3.2	0
923	lterative quantum algorithm for combinatorial optimization based on quantum gradient descent. Results in Physics, 2024, 56, 107204.	4.1	1
924	Universal Generalization of Density Functional Theory for Static Correlation. Physical Review Letters, 2023, 131, .	7.8	1
925	Phonons from Density-Functional Perturbation Theory using the All-Electron Full-Potential Linearized Augmented Plane-Wave Method FLEUR. Electronic Structure, 0, , .	2.8	0
926	Deep Charge: Deep learning model of electron density from a one-shot density functional theory calculation. Physical Review B, 2023, 108, .	3.2	0
927	Entropic Density Functional Theory. Entropy, 2024, 26, 10.	2.2	0
928	Cn, CnH and their anions: Quest for linearity with nâ‰8 even versus odd, and beyond. International Journal of Quantum Chemistry, 2024, 124, .	2.0	0
929	Nanoparticles anchored strategy to develop 2D MoS2 and MoSe2 based room temperature chemiresistive gas sensors. Coordination Chemistry Reviews, 2024, 503, 215657.	18.8	2
930	Benchmarking the accuracy of the separable resolution of the identity approach for correlated methods in the numeric atom-centered orbitals framework. Journal of Chemical Physics, 2024, 160, .	3.0	0
931	Recent advances in smart hydrogels and carbonaceous nanoallotropes composites. Applied Materials Today, 2024, 36, 102058.	4.3	0
932	Photothermal conversion mechanism of the dibenzotetrathiafulvalene-tetracyanobenzene cocrystal based on the transitions between the ground and excited states. Science China Materials, 2024, 67, 242-250.	6.3	0
933	Mo-based MXenes: Synthesis, properties, and applications. Advances in Colloid and Interface Science, 2024, 324, 103077.	14.7	8
934	Nb2CO2 as a promising sensor and adsorbent to capture H2CO gas. Ceramics International, 2024, 50, 12222-12236.	4.8	0
935	Nonvolatile Memristive Materials and Physical Modeling for Inâ€Memory and Inâ€Sensor Computing. Small Science, 2024, 4, .	9.9	0
936	Analysis of two overlapping fragmentation approaches in density matrix construction: GMBE-DM <i>vs.</i> ADMA. Physical Chemistry Chemical Physics, 2024, 26, 4386-4394.	2.8	0
937	Spectral approximation scheme for a hybrid, spin-density Kohn–Sham density-functional theory in an external (nonuniform) magnetic field and a collinear exchange-correlation energy. Journal of Mathematical Chemistry, 2024, 62, 711-760.	1.5	0
938	First-principles study of structural, mechanical, electronic properties and Debye temperature of NbCo2 Laves phases under pressure. Physica B: Condensed Matter, 2024, 676, 415683.	2.7	0
939	Orbital-free quasidensity functional theory. Physical Review Research, 2024, 6, .	3.6	1

#	Article	IF	CITATIONS
940	Variance extrapolation method for neural-network variational Monte Carlo. Machine Learning: Science and Technology, 2024, 5, 015016.	5.0	0
941	xmins:mmi="http://www.w3.org/1998/Math/MathML" altimg="si110.svg" display="inline" id="d1e429"> <mml:msub><mml:mrow></mml:mrow><mml:mrow><mml:mn>2</mml:mn></mml:mrow></mml:msub> MnAl, Pd <mml:math <="" altimg="si110.svg" display="inline" td="" xmlns:mml="http://www.w3.org/1998/Math/MathML"><td>2.3</td><td>0</td></mml:math>	2.3	0
942	Efficient photocatalytic overall water splitting for hydrogen evolution and CO2 reduction with SiCP4 allotrope monolayers. Applied Surface Science, 2024, 654, 159440.	6.1	0
943	Investigating Data Reusability in Density Functional Theory Studies. , 2023, , .		0
944	Understanding 2D Semiconductor Edges by Combining Local and Nonlocal Effects: The Case of MoSi ₂ N ₄ . Chemistry of Materials, 2024, 36, 1526-1535.	6.7	0
945	On-site and intersite Hubbard corrections in magnetic monolayers: The case of <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:msub><mml:mi>FePS</mml:mi><mml:mi><mml:mi><mml:mi><mml:mi><mml:mi><mml:mi><mml:mi><mml:mi><mml:mi><mml:mi><mml:mi><mml:mi><mml:mi><mml:mi><mml:mi><mml:mi><mml:mi><mml:mi><mml:mi><mml:mi><mml:mi><mml:mi><mml:mi><mml:mi><mml:mi><mml:mi><mml:mi><mml:mi><mml:mi><mml:mi><mml:mi><mml:mi><mml:mi><mml:mi><mml:mi><mml:mi><mml:mi><mml:mi><mml:mi><mml:mi><mml:mi><mml:mi><mml:mi><mml:mi><mml:mi><mml:mi><mml:mi><mml:mi><mml:mi><mml:mi><mml:mi><mml:mi><mml:mi><mml:mi><mml:mi><mml:mi><mml:mi><mml:mi><mml:mi><mml:mi><mml:mi><mml:mi><mml:mi><mml:mi><mml:mi><mml:mi><mml:mi><mml:mi><mml:mi><mml:mi><mml:mi><mml:mi><mml:mi><mml:mi><mml:mi><mml:mi><mml:mi><mml:mi><mml:mi><mml:mi><mml:mi><mml:mi><mml:mi><mml:mi><mml:mi><mml:mi><mml:mi><mml:mi><mml:mi><mml:mi><mml:mi><mml:mi><mml:mi><mml:mi><mml:mi><mml:mi><mml:mi><mml:mi><mml:mi><mml:mi><mml:mi><mml:mi><mml:mi><mml:mi><mml:mi><mml:mi><mml:mi><mml:mi><mml:mi><mml:mi><mml:mi><mml:mi><mml:mi><mml:mi><mml:mi><mml:mi><mml:mi><mml:mi><mml:mi><mml:mi><mml:mi><mml:mi><mml:mi><mml:mi><mml:mi><mml:mi><mml:mi><mml:mi><mml:mi><mml:mi><mml:mi><mml:mi><mml:mi><mml:mi><mml:mi><mml:mi><mml:mi><mml:mi><mml:mi><mml:mi><mml:mi><mml:mi><mml:mi><mml:mi><mml:mi><mml:mi><mml:mi><mml:mi><mml:mi><mml:mi><mml:mi><mml:mi><mml:mi><mml:mi><mml:mi><mml:mi><mml:mi><mml:mi><mml:mi><mml:mi><mml:mi><mml:mi><mml:mi><mml:mi><mml:mi><mml:mi><mml:mi><mml:mi><mml:mi><mml:mi><mml:mi><mml:mi><mml:mi><mml:mi><mml:mi><mml:mi><mml:mi><mml:mi><mml:mi><mml:mi><mml:mi><mml:mi><mml:mi><mml:mi><mml:mi><mml:mi><mml:mi><mml:mi><mml:mi><mml:mi><mml:mi><mml:mi><mml:mi><mml:mi><mml:mi><mml:mi><mml:mi><mml:mi><mml:mi><mml:mi><mml:mi><mml:mi><mml:mi><mml:mi><mml:mi><mml:mi><mml:mi><mml:mi><mml:mi><mml:mi><mml:mi><mml:mi><mml:mi><mml:mi><mml:mi><mml:mi><mml:mi><mml:mi><mml:mi><mml:mi><mml:mi><mml:mi><mml:mi><mml:mi><mml:mi><mml:mi><mml:mi><mml:mi><mml:mi><mml:mi><mml:mi><mml:mi><mml:mi><mml:mi><mml:mi></mml:mi></mml:mi></mml:mi></mml:mi></mml:mi></mml:mi></mml:mi></mml:mi></mml:mi></mml:mi></mml:mi></mml:mi></mml:mi></mml:mi></mml:mi></mml:mi></mml:mi></mml:mi></mml:mi></mml:mi></mml:mi></mml:mi></mml:mi></mml:mi></mml:mi></mml:mi></mml:mi></mml:mi></mml:mi></mml:mi></mml:mi></mml:mi></mml:mi></mml:mi></mml:mi></mml:mi></mml:mi></mml:mi></mml:mi></mml:mi></mml:mi></mml:mi></mml:mi></mml:mi></mml:mi></mml:mi></mml:mi></mml:mi></mml:mi></mml:mi></mml:mi></mml:mi></mml:mi></mml:mi></mml:mi></mml:mi></mml:mi></mml:mi></mml:mi></mml:mi></mml:mi></mml:mi></mml:mi></mml:mi></mml:mi></mml:mi></mml:mi></mml:mi></mml:mi></mml:mi></mml:mi></mml:mi></mml:mi></mml:mi></mml:mi></mml:mi></mml:mi></mml:mi></mml:mi></mml:mi></mml:mi></mml:mi></mml:mi></mml:mi></mml:mi></mml:mi></mml:mi></mml:mi></mml:mi></mml:mi></mml:mi></mml:mi></mml:mi></mml:mi></mml:mi></mml:mi></mml:mi></mml:mi></mml:mi></mml:mi></mml:mi></mml:mi></mml:mi></mml:mi></mml:mi></mml:mi></mml:mi></mml:mi></mml:mi></mml:mi></mml:mi></mml:mi></mml:mi></mml:mi></mml:mi></mml:mi></mml:mi></mml:mi></mml:mi></mml:mi></mml:mi></mml:mi></mml:mi></mml:mi></mml:mi></mml:mi></mml:mi></mml:mi></mml:mi></mml:mi></mml:mi></mml:mi></mml:mi></mml:mi></mml:mi></mml:mi></mml:mi></mml:mi></mml:mi></mml:mi></mml:mi></mml:mi></mml:mi></mml:mi></mml:mi></mml:mi></mml:mi></mml:mi></mml:mi></mml:mi></mml:mi></mml:mi></mml:mi></mml:mi></mml:mi></mml:mi></mml:mi></mml:mi></mml:mi></mml:mi></mml:mi></mml:mi></mml:mi></mml:mi></mml:mi></mml:mi></mml:mi></mml:mi></mml:mi></mml:mi></mml:mi></mml:mi></mml:mi></mml:mi></mml:mi></mml:mi></mml:mi></mml:mi></mml:mi></mml:mi></mml:mi></mml:mi></mml:mi></mml:mi></mml:mi></mml:mi></mml:mi></mml:mi></mml:mi></mml:mi></mml:mi></mml:mi></mml:mi></mml:mi></mml:mi></mml:mi></mml:mi></mml:mi></mml:mi></mml:mi></mml:mi></mml:mi></mml:mi></mml:mi></mml:mi></mml:mi></mml:mi></mml:mi></mml:mi></mml:mi></mml:mi></mml:mi></mml:mi></mml:mi></mml:mi></mml:mi></mml:mi></mml:mi></mml:mi></mml:mi></mml:mi></mml:mi></mml:mi></mml:mi></mml:mi></mml:mi></mml:mi></mml:mi></mml:mi></mml:mi></mml:mi></mml:mi></mml:mi></mml:mi></mml:mi></mml:msub></mml:math>	2.4	0
946	Physical Review Materials, 2024, 8, . Machine Learning Enabled Prediction of High Stiffness 2D Materials., 2024, 6, 729-736.		0
947	<i>Ab Initio</i> Path Integral Monte Carlo Simulations of the Uniform Electron Gas on Large Length Scales. Journal of Physical Chemistry Letters, 2024, 15, 1305-1313.	4.6	1
948	Unveiling fructose and glucose binding to human serum albumin: fluorescence measurements and docking, molecular dynamics and quantum biochemistry computations. Journal of Biomolecular Structure and Dynamics, 0, , 1-21.	3.5	0
949	High spin polarization in quaternary Heusler Fe–Rh–Mn–Al alloys. Physica B: Condensed Matter, 2024, 677, 415736.	2.7	0
950	From NdNiO ₂ to a Mott Multiferroic BiNiO ₂ . Ferroelectrics, Letters Section, 2024, 51, 31-44.	1.0	0
951	Transferable empirical pseudopotenials from machine learning. Physical Review B, 2024, 109, .	3.2	0
952	How close are the classical two-body potentials to $\langle i \rangle$ abÂinitio $\langle i \rangle$ calculations? Insights from linear machine learning based force matching. Journal of Chemical Physics, 2024, 160, .	3.0	0
953	Twisted van der Waals Quantum Materials: Fundamentals, Tunability, and Applications. Chemical Reviews, 2024, 124, 1992-2079.	47.7	0
954	Negative differential friction in van der Waals layered materials: The role of interlayer quasibonding repulsion. Physical Review B, 2024, 109, .	3.2	0
955	Synthesis of metal–organic frameworks with multiple nitrogen groups for selective capturing Ag(I) from wastewater. Journal of Colloid and Interface Science, 2024, 663, 761-774.	9.4	0
956	Extracting many-body quantum resources within one-body reduced density matrix functional theory. Physical Review Research, 2024, 6, .	3.6	0
957	Comprehensive First-Principles Modeling of Experimentally Synthesized BiPO ₄ Polymorphs. Journal of Physical Chemistry C, 2024, 128, 4779-4788.	3.1	0

#	Article	IF	CITATIONS
958	tightbinder: A Python package for semi-empirical tight-binding models of crystalline and disordered solids. Journal of Open Source Software, 2024, 9, 5810.	4.6	0
959	Unified understanding to the rich electronic-structure evolutions of two-dimensional black phosphorus under pressure. Physical Review Research, 2024, 6, .	3.6	0
960	First-principles study on the effects of fast neutron irradiation and fast neutron irradiation under the external electric field on carbon-based material AB bilayer graphene. Diamond and Related Materials, 2024, 144, 110988.	3.9	0
961	Work Function Prediction by Graph Neural Networks for Configurationally Hybridized Boron-Doped Graphene. Langmuir, 2024, 40, 7087-7094.	3.5	0
962	Electron-beam-based Compton scattering x-ray source for probing high-energy-density physics. Physical Review Accelerators and Beams, 2024, 27, .	1.6	0