

Eberhard K U Gross

List of Publications by Year in descending order

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255
papers

29,567
citations

11608

70
h-index

4978

167
g-index

258
all docs

258
docs citations

258
times ranked

16904
citing authors

#	ARTICLE	IF	CITATIONS
1	Density-Functional Theory for Time-Dependent Systems. <i>Physical Review Letters</i> , 1984, 52, 997-1000.	2.9	7,180
2	Excitation Energies from Time-Dependent Density-Functional Theory. <i>Physical Review Letters</i> , 1996, 76, 1212-1215.	2.9	1,466
3	Reproducibility in density functional theory calculations of solids. <i>Science</i> , 2016, 351, aad3000.	6.0	1,113
4	TIME-DEPENDENT DENSITY FUNCTIONAL THEORY. <i>Annual Review of Physical Chemistry</i> , 2004, 55, 427-455.	4.8	1,099
5	Time-Dependent Density-Functional Theory. <i>Advances in Quantum Chemistry</i> , 1990, 21, 255-291.	0.4	992
6	Local density-functional theory of frequency-dependent linear response. <i>Physical Review Letters</i> , 1985, 55, 2850-2852.	2.9	939
7	Time-dependent density functional theory: Past, present, and future. <i>Journal of Chemical Physics</i> , 2005, 123, 062206.	1.2	791
8	octopus: a tool for the application of time-dependent density functional theory. <i>Physica Status Solidi (B): Basic Research</i> , 2006, 243, 2465-2488.	0.7	756
9	Density functional theory of time-dependent phenomena. , 1996, , 81-172.		476
10	Understanding band gaps of solids in generalized Kohn-Sham theory. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2017, 114, 2801-2806.	3.3	423
11	Fundamentals of Time-Dependent Density Functional Theory. <i>Lecture Notes in Physics</i> , 2012, , .	0.3	370
12	Exact Coulomb cutoff technique for supercell calculations. <i>Physical Review B</i> , 2006, 73, .	1.1	369
13	Density-Functional Theory for Superconductors. <i>Physical Review Letters</i> , 1988, 60, 2430-2433.	2.9	362
14	How to represent crystal structures for machine learning: Towards fast prediction of electronic properties. <i>Physical Review B</i> , 2014, 89, .	1.1	353
15	Exact Factorization of the Time-Dependent Electron-Nuclear Wave Function. <i>Physical Review Letters</i> , 2010, 105, 123002.	2.9	351
16	Quantum optimal control theory. <i>Journal of Physics B: Atomic, Molecular and Optical Physics</i> , 2007, 40, R175-R211.	0.6	330
17	Ab initio theory of superconductivity. I. Density functional formalism and approximate functionals. <i>Physical Review B</i> , 2005, 72, .	1.1	314
18	Density-functional theory for ensembles of fractionally occupied states. I. Basic formalism. <i>Physical Review A</i> , 1988, 37, 2809-2820.	1.0	301

#	ARTICLE	IF	CITATIONS
19	Time-dependent quantum transport: A practical scheme using density functional theory. Physical Review B, 2005, 72, .	1.1	291
20	Rayleigh-Ritz variational principle for ensembles of fractionally occupied states. Physical Review A, 1988, 37, 2805-2808.	1.0	281
21	Intense-Field Double Ionization of Helium: Identifying the Mechanism. Physical Review Letters, 2000, 85, 4707-4710.	2.9	278
22	Ab initio theory of superconductivity. II. Application to elemental metals. Physical Review B, 2005, 72, .	1.1	261
23	Density-functional theory for ensembles of fractionally occupied states. II. Application to the He atom. Physical Review A, 1988, 37, 2821-2833.	1.0	237
24	Time-Dependent Optimized Effective Potential. Physical Review Letters, 1995, 74, 872-875.	2.9	222
25	Multicomponent Density-Functional Theory for Electrons and Nuclei. Physical Review Letters, 2001, 86, 2984-2987.	2.9	206
26	Ab Initio Description of High-Temperature Superconductivity in Dense Molecular Hydrogen. Physical Review Letters, 2008, 100, 257001.	2.9	199
27	Correlated electron-nuclear dynamics: Exact factorization of the molecular wavefunction. Journal of Chemical Physics, 2012, 137, 22A530.	1.2	198
28	Laser-Induced Demagnetization at Ultrashort Time Scales: Predictions of TDDFT. Journal of Chemical Theory and Computation, 2015, 11, 4870-4874.	2.3	167
29	Bootstrap Approximation for the Exchange-Correlation Kernel of Time-Dependent Density-Functional Theory. Physical Review Letters, 2011, 107, 186401.	2.9	164
30	Superconductivity in Lithium, Potassium, and Aluminum under Extreme Pressure: A First-Principles Study. Physical Review Letters, 2006, 96, 047003.	2.9	159
31	Excitations in Time-Dependent Density-Functional Theory. Physical Review Letters, 2003, 90, 043005.	2.9	156
32	High temperature superconductivity in sulfur and selenium hydrides at high pressure. European Physical Journal B, 2016, 89, 1.	0.6	154
33	Spin-Density Functionals from Current-Density Functional Theory and Vice Versa: A Road towards New Approximations. Physical Review Letters, 1997, 78, 1872-1875.	2.9	141
34	Density-functional theory using an optimized exchange-correlation potential. Chemical Physics Letters, 1995, 240, 141-150.	1.2	140
35	Reduced density matrix functional for many-electron systems. Physical Review B, 2008, 78, .	1.1	138
36	Superconducting Properties of MgB ₂ from First Principles. Physical Review Letters, 2005, 94, 037004.	2.9	137

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37	Coupled-Trajectory Quantum-Classical Approach to Electronic Decoherence in Nonadiabatic Processes. <i>Physical Review Letters</i> , 2015, 115, 073001.	2.9	126
38	Adiabatic Approximation in Nonperturbative Time-Dependent Density-Functional Theory. <i>Physical Review Letters</i> , 2008, 100, 153004.	2.9	125
39	Superconductivity in metastable phases of phosphorus-hydride compounds under high pressure. <i>Physical Review B</i> , 2016, 93, .	1.1	125
40	Ab Initio Nonadiabatic Dynamics with Coupled Trajectories: A Rigorous Approach to Quantum (De)Coherence. <i>Journal of Physical Chemistry Letters</i> , 2017, 8, 3048-3055.	2.1	123
41	Time-dependent electron localization function. <i>Physical Review A</i> , 2005, 71, .	1.0	122
42	Quantum-Classical Nonadiabatic Dynamics: Coupled- vs Independent-Trajectory Methods. <i>Journal of Chemical Theory and Computation</i> , 2016, 12, 2127-2143.	2.3	117
43	Time-dependent approach to electron pumping in open quantum systems. <i>Physical Review B</i> , 2008, 77, .	1.1	115
44	Dynamical Coulomb Blockade and the Derivative Discontinuity of Time-Dependent Density Functional Theory. <i>Physical Review Letters</i> , 2010, 104, 236801.	2.9	115
45	Electron correlation energies from scaled exchange-correlation kernels: Importance of spatial versus temporal nonlocality. <i>Physical Review B</i> , 2000, 61, 13431-13437.	1.1	113
46	Toward the description of van der Waals interactions within density functional theory. <i>Journal of Computational Chemistry</i> , 1999, 20, 12-22.	1.5	106
47	Even-Harmonic Generation due to Beyond-Born-Oppenheimer Dynamics. <i>Physical Review Letters</i> , 2001, 87, 103901.	2.9	105
48	Optimal Control of Quantum Rings by Terahertz Laser Pulses. <i>Physical Review Letters</i> , 2007, 98, 157404.	2.9	102
49	Anisotropic gap of superconducting CaC ₆ : A first-principles density functional calculation. <i>Physical Review B</i> , 2007, 75, .	1.1	101
50	Time-Dependent Density Functional Theory beyond Linear Response: An Exchange-Correlation Potential with Memory. <i>Physical Review Letters</i> , 1997, 79, 1905-1908.	2.9	99
51	Thermal conductivity in PbTe from first principles. <i>Physical Review B</i> , 2015, 91, .	1.1	98
52	Strong-field ionization dynamics of a model H ₂ molecule. <i>Physical Review A</i> , 2002, 65, .	1.0	97
53	Spurious Interactions, and Their Correction, in the Ensemble-Kohn-Sham Scheme for Excited States. <i>Physical Review Letters</i> , 2002, 88, 033003.	2.9	94
54	Dynamical Steps that Bridge Piecewise Adiabatic Shapes in the Exact Time-Dependent Potential Energy Surface. <i>Physical Review Letters</i> , 2013, 110, 263001.	2.9	94

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55	Is the Molecular Berry Phase an Artifact of the Born-Oppenheimer Approximation?. Physical Review Letters, 2014, 113, 263004.	2.9	93
56	Local Density-Functional Theory of Frequency-Dependent Linear Response. Physical Review Letters, 1986, 57, 923-923.	2.9	91
57	Density-matrix-power functional: Performance for finite systems and the homogeneous electron gas. Physical Review A, 2009, 79, .	1.0	91
58	The exact forces on classical nuclei in non-adiabatic charge transfer. Journal of Chemical Physics, 2015, 142, 084303.	1.2	83
59	Vibrational properties of MnO and NiO from DFT U -based density functional perturbation theory. Physical Review B, 2011, 84, .	1.1	82
60	Ab initio angle- and energy-resolved photoelectron spectroscopy with time-dependent density-functional theory. Physical Review A, 2012, 85, .	1.0	82
61	Electronic non-adiabatic states: towards a density functional theory beyond the Born-Oppenheimer approximation. Philosophical Transactions Series A, Mathematical, Physical, and Engineering Sciences, 2014, 372, 20130059.	1.6	80
62	The 2021 room-temperature superconductivity roadmap. Journal of Physics Condensed Matter, 2022, 34, 183002.	0.7	79
63	Discontinuities of the exchange-correlation kernel and charge-transfer excitations in time-dependent density-functional theory. Physical Review A, 2012, 85, .	1.0	77
64	Correlation effects on the third-frequency-moment sum rule of electron liquids. Physical Review B, 1987, 35, 3003-3004.	1.1	76
65	Molecular excitation energies from time-dependent density functional theory. Computational and Theoretical Chemistry, 2000, 501-502, 353-367.	1.5	76
66	First-Principles Approach to Noncollinear Magnetism: Towards Spin Dynamics. Physical Review Letters, 2007, 98, 196405.	2.9	74
67	Two-band superconductivity in Pb from ab initio calculations. Physical Review B, 2007, 75, .	1.1	73
68	Exact Conditions in Finite-Temperature Density-Functional Theory. Physical Review Letters, 2011, 107, 163001.	2.9	73
69	Correlation potentials for molecular bond dissociation within the self-consistent random phase approximation. Journal of Chemical Physics, 2012, 136, 034106.	1.2	72
70	Controlling the Dynamics of Many-Electron Systems from First Principles: A Combination of Optimal Control and Time-Dependent Density-Functional Theory. Physical Review Letters, 2012, 109, 153603.	2.9	72
71	Ab initio Eliashberg Theory: Making Genuine Predictions of Superconducting Features. Journal of the Physical Society of Japan, 2018, 87, 041012.	0.7	72
72	Multicomponent density-functional theory for electrons and nuclei. Physical Review A, 2008, 78, .	1.0	70

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73	Time-Dependent Density-Functional Theory for Superconductors. <i>Physical Review Letters</i> , 1994, 73, 2915-2918.	2.9	68
74	Exact-exchange density-functional calculations for noble-gas solids. <i>Physical Review B</i> , 2004, 69, .	1.1	68
75	Nuclear velocity perturbation theory for vibrational circular dichroism: An approach based on the exact factorization of the electron-nuclear wave function. <i>Journal of Chemical Physics</i> , 2015, 143, 074106.	1.2	67
76	Optimal control of time-dependent targets. <i>Physical Review A</i> , 2005, 71, .	1.0	66
77	Gradient expansion of the Coulomb exchange energy. <i>Zeitschrift für Physik A</i> , 1981, 302, 103-106.	1.4	65
78	Density Functional Theory of Time-Dependent Systems. <i>NATO ASI Series Series B: Physics</i> , 1995, , 149-171.	0.2	65
79	Spectral Density and Metal-Insulator Phase Transition in Mott Insulators within Reduced Density Matrix Functional Theory. <i>Physical Review Letters</i> , 2013, 110, 116403.	2.9	65
80	Comparative study of many-body perturbation theory and time-dependent density functional theory in the out-of-equilibrium Anderson model. <i>Physical Review B</i> , 2011, 84, .	1.1	61
81	Electron-phonon interaction and superconductivity in metallic molecular hydrogen. II. Superconductivity under pressure. <i>Physical Review B</i> , 2010, 81, .	1.1	60
82	Ultrafast laser induced local magnetization dynamics in Heusler compounds. <i>Scientific Reports</i> , 2016, 6, 38911.	1.6	60
83	Thomas-Fermi approach to diatomic systems. I. Solution of the Thomas-Fermi and Thomas-Fermi-Dirac-Weizsäcker equations. <i>Physical Review A</i> , 1979, 20, 1798-1807.	1.0	59
84	The optimized effective potential method of density functional theory: Applications to atomic and molecular systems. <i>International Journal of Quantum Chemistry</i> , 1997, 64, 95-110.	1.0	57
85	Excitation energies from time-dependent density functional theory using exact and approximate potentials. <i>International Journal of Quantum Chemistry</i> , 2000, 80, 534-554.	1.0	57
86	Mixed quantum-classical dynamics from the exact decomposition of electron-nuclear motion. <i>Europhysics Letters</i> , 2014, 106, 33001.	0.7	57
87	Classical nuclear motion coupled to electronic non-adiabatic transitions. <i>Journal of Chemical Physics</i> , 2014, 141, 214101.	1.2	54
88	Molecular geometric phase from the exact electron-nuclear factorization. <i>Physical Review A</i> , 2016, 93, .	1.0	54
89	Large magnetocrystalline anisotropy in tetragonally distorted Heuslers: a systematic study. <i>Journal Physics D: Applied Physics</i> , 2017, 50, 095002.	1.3	52
90	Mixed quantum-classical dynamics on the exact time-dependent potential energy surface: a fresh look at non-adiabatic processes. <i>Molecular Physics</i> , 2013, 111, 3625-3640.	0.8	51

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91	Exact Factorization-Based Density Functional Theory of Electrons and Nuclei. <i>Physical Review Letters</i> , 2016, 117, 193001.	2.9	50
92	The optimal one dimensional periodic table: a modified Pettifor chemical scale from data mining. <i>New Journal of Physics</i> , 2016, 18, 093011.	1.2	50
93	Performance of one-body reduced density-matrix functionals for the homogeneous electron gas. <i>Physical Review B</i> , 2007, 75, .	1.1	49
94	Competing Spin Transfer and Dissipation at $\langle \text{mml:math display="inline"><mml:mrow><mml:mi>Co</mml:mi><mml:mo>/</mml:mo><mml:mi>Cu</mml:mi><mml:mo>stretchy="false"></mml:mo><mml:mn>001</mml:mn><mml:mo>Tj ETQq0 0 0 rgBT /Overlock 10 Tf 50 612 Td (stretchy="false"></mml:mo></mml:math>$	2.9	48
95	Physical Review Letters, 2019, 122, 067202. Electron-phonon interaction and superconductivity in metallic molecular hydrogen. I. Electronic and dynamical properties under pressure. <i>Physical Review B</i> , 2010, 81, .	1.1	47
96	Transverse Spin-Gradient Functional for Noncollinear Spin-Density-Functional Theory. <i>Physical Review Letters</i> , 2013, 111, 156401.	2.9	47
97	Tailoring laser pulses with spectral and fluence constraints using optimal control theory. <i>Journal of Optics B: Quantum and Semiclassical Optics</i> , 2005, 7, S300-S312.	1.4	46
98	Superconducting properties of MgB2 from first principles. <i>Physica C: Superconductivity and Its Applications</i> , 2007, 456, 45-53.	0.6	46
99	Superconducting pairing mediated by spin fluctuations from first principles. <i>Physical Review B</i> , 2014, 90, .	1.1	46
100	Current density functional theory of spontaneously magnetised solids. <i>Europhysics Letters</i> , 1997, 40, 545-550.	0.7	44
101	Electronic Flux Density beyond the Born- ϵ -Oppenheimer Approximation. <i>Journal of Physical Chemistry A</i> , 2016, 120, 3316-3325.	1.1	44
102	An efficient algorithm for time propagation as applied to linearized augmented plane wave method. <i>Computer Physics Communications</i> , 2016, 209, 92-95.	3.0	43
103	How Interatomic Steps in the Exact Kohn- ϵ -Sham Potential Relate to Derivative Discontinuities of the Energy. <i>Journal of Physical Chemistry Letters</i> , 2017, 8, 5974-5980.	2.1	43
104	Ultrafast demagnetization in bulk versus thin films: an <i>ab initio</i> study. <i>Journal of Physics Condensed Matter</i> , 2017, 29, 224001.	0.7	42
105	Accurate solution of the Thomas-Fermi-Dirac-Weizsäcker variational equations for the case of neutral atoms and positive ions. <i>Zeitschrift für Physik A</i> , 1982, 309, 5-11.	1.4	41
106	Scaling and virial theorems in current-density-functional theory. <i>Physical Review A</i> , 1996, 53, R5-R8.	1.0	41
107	Open shells in reduced-density-matrix-functional theory. <i>Physical Review A</i> , 2005, 72, .	1.0	41
108	<i>Ab initio</i> prediction of pressure-induced superconductivity in potassium. <i>Physical Review B</i> , 2006, 73, .	1.1	41

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109	Reversible Formation of 2D Electron Gas at the LaFeO ₃ /SrTiO ₃ Interface via Control of Oxygen Vacancies. <i>Advanced Materials</i> , 2017, 29, 1604447.	11.1	41
110	Electronic Schrödinger equation with nonclassical nuclei. <i>Physical Review A</i> , 2014, 89, .	1.0	40
111	Laser-induced electron localization in H ₂ ⁺ : mixed quantum-classical dynamics based on the exact time-dependent potential energy surface. <i>Physical Chemistry Chemical Physics</i> , 2015, 17, 29271-29280.	1.3	40
112	An exact factorization perspective on quantum interferences in nonadiabatic dynamics. <i>Journal of Chemical Physics</i> , 2016, 145, 034103.	1.2	40
113	Orbital magnetism in the density functional theory of superconductors. <i>Journal De Physique</i> , 1989, 50, 2601-2612.	1.8	40
114	Local Density Approximation for Superconductors. <i>Physical Review Letters</i> , 1999, 83, 2628-2631.	2.9	39
115	Electronic Structure via Potential Functional Approximations. <i>Physical Review Letters</i> , 2011, 106, 236404.	2.9	39
116	Exact Single-Electron Approach to the Dynamics of Molecules in Strong Laser Fields. <i>Physical Review Letters</i> , 2017, 118, 163202.	2.9	39
117	Time-dependent natural orbitals and occupation numbers. <i>Europhysics Letters</i> , 2010, 92, 23001.	0.7	38
118	Correlation effects in bistability at the nanoscale: Steady state and beyond. <i>Physical Review B</i> , 2012, 85, .	1.1	38
119	Time-dependent electron localization functions for coupled nuclear-electronic motion. <i>Journal of Chemical Physics</i> , 2004, 121, 9666-9670.	1.2	37
120	Discontinuity of the chemical potential in reduced-density-matrix-functional theory. <i>Europhysics Letters</i> , 2007, 77, 67003.	0.7	37
121	Local Measurement of the Eliashberg Function of Pb Islands: Enhancement of Electron-Phonon Coupling by Quantum Well States. <i>Physical Review Letters</i> , 2015, 114, 047002.	2.9	37
122	Bound states in time-dependent quantum transport: oscillations and memory effects in current and density. <i>Physical Chemistry Chemical Physics</i> , 2009, 11, 4535.	1.3	36
123	Response to "Comment on "Correlated electron-nuclear dynamics: Exact factorization of the molecular wavefunction" [J. Chem. Phys. 139, 087101 (2013)]. <i>Journal of Chemical Physics</i> , 2013, 139, 087102.	1.2	36
124	Discontinuities of the Chemical Potential in Reduced Density Matrix Functional Theory. <i>Zeitschrift Fur Physikalische Chemie</i> , 2010, 224, 467-480.	1.4	35
125	Ab initio theory of iron-based superconductors. <i>Physical Review B</i> , 2016, 94, .	1.1	35
126	Ensemble-Density functional theory for excited states. <i>International Journal of Quantum Chemistry</i> , 1990, 38, 707-716.	1.0	34

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127	Relativistic framework for microscopic theories of superconductivity. I. The Dirac equation for superconductors. <i>Physical Review B</i> , 1999, 59, 7140-7154.	1.1	34
128	Exchange-energy functionals for finite two-dimensional systems. <i>Physical Review B</i> , 2007, 76, .	1.1	34
129	Femtosecond laser pulse shaping for enhanced ionization. <i>Europhysics Letters</i> , 2009, 87, 53001.	0.7	34
130	Enhancing and controlling single-atom high-harmonic generation spectra: a time-dependent density-functional scheme. <i>European Physical Journal B</i> , 2015, 88, 1.	0.6	34
131	Optimal control of laser-induced spin-orbit mediated ultrafast demagnetization. <i>New Journal of Physics</i> , 2016, 18, 013014.	1.2	34
132	Multicomponent density-functional theory for time-dependent systems. <i>Physical Review A</i> , 2007, 76, .	1.0	33
133	On the mechanism of strong-field double photoionization in the helium atom. <i>Journal of Physics B: Atomic, Molecular and Optical Physics</i> , 2000, 33, 433-442.	0.6	32
134	Optimal laser control of double quantum dots. <i>Physical Review B</i> , 2008, 77, .	1.1	32
135	Electronic, vibrational, and superconducting properties of CaBeSi : First-principles calculations. <i>Physical Review B</i> , 2009, 79, .	1.1	32
136	A functional of the one-body-reduced density matrix derived from the homogeneous electron gas: Performance for finite systems. <i>Journal of Chemical Physics</i> , 2009, 130, 064109.	1.2	32
137	The role of Coulomb interaction in the superconducting properties of CaC_6 and H under pressure. <i>Superconductor Science and Technology</i> , 2009, 22, 034006.	1.8	32
138	Time-dependent density-functional and reduced density-matrix methods for few electrons: Exact versus adiabatic approximations. <i>Chemical Physics</i> , 2011, 391, 1-10.	0.9	32
139	Semiclassical analysis of the electron-nuclear coupling in electronic non-adiabatic processes. <i>Annalen Der Physik</i> , 2015, 527, 546-555.	0.9	32
140	Spin-multiplet energies from time-dependent density functional theory. <i>International Journal of Quantum Chemistry</i> , 1996, 60, 1393-1401.	1.0	29
141	Asymptotic Properties of the Optimized Effective Potential. <i>Advances in Quantum Chemistry</i> , 1998, , 31-48.	0.4	29
142	Resonant inelastic soft x-ray scattering of Be chalcogenides. <i>Physical Review B</i> , 2006, 73, .	1.1	29
143	The role of bound states in time-dependent quantum transport. <i>Applied Physics A: Materials Science and Processing</i> , 2008, 93, 355-364.	1.1	29
144	Phononic self-energy effects and superconductivity in CaC_6 . <i>Physical Review B</i> , 2012, 85, .	1.1	29

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145	Paramagnons in FeSe close to a magnetic quantum phase transition: Ab initio study. Physical Review B, 2012, 86, .	1.1	29
146	Reduced-density-matrix-functional theory at finite temperature: Theoretical foundations. Physical Review A, 2015, 92, .	1.0	29
147	Optimization schemes for selective molecular cleavage with tailored ultrashort laser pulses. Chemical Physics, 2011, 391, 50-61.	0.9	28
148	Discrete peaks in above-threshold double-ionization spectra. Physical Review A, 2001, 64, .	1.0	27
149	Gaussian approximations for the exchange-energy functional of current-carrying states: Applications to two-dimensional systems. Physical Review A, 2009, 80, .	1.0	27
150	A guided tour of time-dependent density functional theory. , 1998, , 116-146.		26
151	Comparison of exact-exchange calculations for solids in current-spin-density- and spin-density-functional theory. Physical Review B, 2007, 76, .	1.1	26
152	Correlation energy of finite two-dimensional systems: Toward nonempirical and universal modeling. Physical Review B, 2009, 79, .	1.1	26
153	Magnon spectrum of transition-metal oxides: Calculations including long-range magnetic interactions using the $\langle \text{mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"} \langle \text{mml:mrow} \langle \text{mml:mi} \text{LSDA} \langle \text{mml:mi} \rangle \langle \text{mml:mo} \rangle + \langle \text{mml:mo} \rangle \langle \text{mml:mi} \rangle U \langle \text{mml:mi} \rangle \langle \text{mml:mrow} \rangle \langle \text{mml:math} \rangle \text{method}$. Physical Review B, 2011, 84, .	1.1	26
154	First-Principles Calculation of the Real-Space Order Parameter and Condensation Energy Density in Phonon-Mediated Superconductors. Physical Review Letters, 2015, 115, 097002.	2.9	26
155	On the Mass of Atoms in Molecules: Beyond the Born-Oppenheimer Approximation. Physical Review X, 2017, 7, .	2.8	26
156	Thomas-Fermi approach to diatomic systems. II. Correlation diagrams for N-N and Ne-Ne. Physical Review A, 1979, 20, 1808-1815.	1.0	25
157	Potential functionals versus density functionals. Physical Review A, 2013, 88, .	1.0	25
158	Ensemble-Hartree-Fock scheme for excited states. The optimized effective potential method. Physica B: Condensed Matter, 2002, 318, 328-332.	1.3	24
159	Time-dependent variational approach to molecules in strong laser fields. Chemical Physics, 2004, 304, 183-202.	0.9	24
160	Optimized effective potential method in current-spin-density-functional theory. Physical Review A, 2006, 74, .	1.0	24
161	Discontinuous functional for linear-response time-dependent density-functional theory: The exact-exchange kernel and approximate forms. Physical Review A, 2013, 88, .	1.0	24
162	Ab initio theory of superconductivity in a magnetic field. I. Spin density functional theory for superconductors and Eliashberg equations. Physical Review B, 2015, 92, .	1.1	24

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163	Electronic exchange in quantum rings: Beyond the local-density approximation. <i>Physical Review B</i> , 2009, 79, .	1.1	23
164	Source-Free Exchange-Correlation Magnetic Fields in Density Functional Theory. <i>Journal of Chemical Theory and Computation</i> , 2018, 14, 1247-1253.	2.3	23
165	Exchange-correlation orbital functionals in current-density functional theory: Application to a quantum dot in magnetic fields. <i>Physical Review B</i> , 2008, 77, .	1.1	22
166	Optimal control of strong-field ionization with time-dependent density-functional theory. <i>Physical Review A</i> , 2013, 88, .	1.0	22
167	Asymptotic analysis of the Berry curvature in the G - W approximation model. <i>Physical Review A</i> , 2017, 96, .		
168	Density functional theory of electron transfer beyond the Born-Oppenheimer approximation: Case study of LiF. <i>Journal of Chemical Physics</i> , 2018, 148, 084110.	1.2	22
169	Relativistic theory of superconductivity. <i>Physics Letters, Section A: General, Atomic and Solid State Physics</i> , 1995, 198, 261-266.	0.9	21
170	Chapter 10 Time-dependent transport phenomena. <i>Theoretical and Computational Chemistry</i> , 2007, 17, 247-284.	0.2	21
171	Discontinuity of the chemical potential in reduced-density-matrix-functional theory for open-shell systems. <i>Physical Review A</i> , 2009, 79, .	1.0	21
172	Optical Response of Extended Systems Using Time-Dependent Density Functional Theory. <i>Topics in Current Chemistry</i> , 2014, 347, 235-257.	4.0	21
173	Multiplicity of solutions to G - W approximations. <i>Physical Review B</i> , 2015, 92, .		
174	Electron-nuclear wave-packet dynamics through a conical intersection. <i>Journal of Chemical Physics</i> , 2017, 146, 074304.	1.2	21
175	Surface hopping in laser-driven molecular dynamics. <i>Physical Review A</i> , 2017, 95, .	1.0	21
176	Density-functional theory of the superconducting state. <i>International Journal of Quantum Chemistry</i> , 1991, 40, 289-297.	1.0	20
177	Conventional Quantum Chemical Correlation Energy Versus Density-Functional Correlation Energy. <i>ACS Symposium Series</i> , 1996, , 42-53.	0.5	20
178	Approximate relativistic optimized potential method. <i>Physical Review A</i> , 1998, 57, 138-148.	1.0	20
179	Relativistic framework for microscopic theories of superconductivity. II. The Pauli equation for superconductors. <i>Physical Review B</i> , 1999, 59, 7155-7165.	1.1	20
180	Theory of Dichroism in the Electromagnetic Response of Superconductors. <i>Physical Review Letters</i> , 1997, 78, 3753-3756.	2.9	18

#	ARTICLE	IF	CITATIONS
181	Theoretical investigation of optical conductivity in $\text{Ba}(\text{Fe}_{1-x}\text{Co}_x)_2\text{As}_2$. <i>Physical Review B</i> , 2011, 83, .	1.1	18
182	<i>Ab initio</i> theory of superconductivity in a magnetic field. II. Numerical solution. <i>Physical Review B</i> , 2015, 92, .	1.1	18
183	Adiabatic Connection and the Kohn-Sham Variety of Potential-Functional Theory. <i>Journal of Chemical Theory and Computation</i> , 2009, 5, 844-849.	2.3	17
184	Enhanced excitonic effects in the energy loss spectra of LiF and Ar at large momentum transfer. <i>New Journal of Physics</i> , 2012, 14, 053052.	1.2	17
185	Spectrum for Nonmagnetic Mott Insulators from Power Functional within Reduced Density Matrix Functional Theory. <i>Journal of Chemical Theory and Computation</i> , 2015, 11, 4895-4899.	2.3	17
186	Exact factorization-based density functional theory of electron-phonon systems. <i>Physical Review B</i> , 2019, 99, .	1.1	17
187	Phase-space analysis of double ionization. <i>Optics Express</i> , 2001, 8, 411.	1.7	16
188	Measuring the Kernel of Time-Dependent Density Functional Theory with X-Ray Absorption Spectroscopy of 3d Transition Metals. <i>Physical Review Letters</i> , 2005, 95, 253006.	2.9	16
189	Electron localization function for two-dimensional systems. <i>Physical Review B</i> , 2008, 77, .	1.1	16
190	Thomas-Fermi potentials for quasimolecular collision processes. <i>Physics Letters, Section A: General, Atomic and Solid State Physics</i> , 1976, 57, 131-134.	0.9	15
191	First-principles study of rare-earth-doped superconducting CaFe_2As_2 . <i>Physical Review B</i> , 2012, 86, .	1.1	15
192	Ionization potentials and electron affinities from reduced-density-matrix functional theory. <i>Physical Review A</i> , 2012, 85, .	1.0	15
193	Density functional theory for superconductors. <i>International Journal of Quantum Chemistry</i> , 2004, 99, 790-797.	1.0	14
194	Magnetism in CeFeAsO and LaFeAsO . <i>Physical Review B</i> , 2009, 80, .	1.1	14
195	Minimization procedure in reduced density matrix functional theory by means of an effective noninteracting system. <i>Computational and Theoretical Chemistry</i> , 2013, 1003, 114-122.	1.1	14
196	Electron-nuclear entanglement in the time-dependent molecular wavefunction. <i>Computational and Theoretical Chemistry</i> , 2019, 1151, 99-106.	1.1	14
197	On the degeneracy of atomic states within exact-exchange (spin-) density functional theory. <i>Journal of Chemical Physics</i> , 2006, 125, 084105.	1.2	13
198	Effect of discontinuities in Kohn-Sham-based chemical reactivity theory. <i>Journal of Chemical Physics</i> , 2012, 136, 114102.	1.2	13

#	ARTICLE	IF	CITATIONS
217	Many-body Green's function theory of electrons and nuclei beyond the Born-Oppenheimer approximation. <i>Physical Review B</i> , 2020, 101, .	1.1	10
218	Noncollinear spin-spiral phase for the uniform electron gas within reduced-density-matrix-functional theory. <i>Physical Review B</i> , 2010, 81, .	1.1	9
219	Solution of the Thomas-Fermi equation for triatomic systems. <i>Journal of Physics B: Atomic and Molecular Physics</i> , 1978, 11, 3795-3802.	1.6	8
220	Zeros of the Frequency-Dependent Linear Density Response. <i>Physical Review Letters</i> , 1988, 61, 1518-1518.	2.9	8
221	Accurate Formula for the Macroscopic Polarization of Strongly Correlated Materials. <i>Journal of Physical Chemistry Letters</i> , 2018, 9, 7045-7051.	2.1	8
222	Model Hamiltonian for strongly correlated systems: Systematic, self-consistent, and unique construction. <i>Physical Review B</i> , 2019, 99, .	1.1	8
223	Fock-Space Embedding Theory: Application to Strongly Correlated Topological Phases. <i>Physical Review Letters</i> , 2021, 127, 116401.	2.9	8
224	Time-Dependent Optimized Effective Potential in the Linear Response Regime. , 1998, , 177-197.		8
225	Extended Thomas-Fermi approach to diatomic systems. <i>Physics Letters, Section A: General, Atomic and Solid State Physics</i> , 1979, 71, 49-53.	0.9	7
226	Exchange-correlation approximations for reduced-density-matrix-functional theory at finite temperature: Capturing magnetic phase transitions in the homogeneous electron gas. <i>Physical Review A</i> , 2017, 96, .	1.0	7
227	Complete description of the magnetic ground state in spinel vanadates. <i>Physical Review B</i> , 2019, 100, .	1.1	7
228	Thomas-Fermi approach to diatomic quasimolecules: Correlation diagrams for neutral, heteronuclear systems. <i>Zeitschrift für Physik A</i> , 1980, 298, 167-171.	1.4	6
229	Frequency-dependent linear response of superconducting systems. <i>International Journal of Quantum Chemistry</i> , 1995, 56, 521-533.	1.0	6
230	Double-pole approximation in time-dependent density functional theory. <i>International Journal of Quantum Chemistry</i> , 2006, 106, 2840-2847.	1.0	6
231	Coherent quantum switch driven by optimized laser pulses. <i>Physica E: Low-Dimensional Systems and Nanostructures</i> , 2008, 40, 1593-1595.	1.3	6
232	Static and dynamical susceptibility of $\text{LaO}_{1-x}\text{FeAs}$. <i>Physical Review B</i> , 2010, 81, .	1.1	6
233	Comment on "Estimating Excitonic Effects in the Absorption Spectra of Solids: Problems and Insight from a Guided Iteration Scheme": <i>Physical Review Letters</i> , 2016, 117, 159701.	2.9	6
234	Multi-state impact parameter approximation for many particle excitations in atomic collisions; Total cross sections for Na-Ne and N-Ne. <i>Zeitschrift für Physik A</i> , 1978, 285, 353-356.	1.4	5

#	ARTICLE	IF	CITATIONS
235	Publisher's Note: <i>Ab initio</i> Description of High-Temperature Superconductivity in Dense Molecular Hydrogen [Phys. Rev. Lett. 100 , 257001 (2008)]. Physical Review Letters, 2008, 101, .	2.9	4
236	L1 ₀ Stacked Binaries as Candidates for Hard Magnets: FePt, MnAl and MnGa. Annalen Der Physik, 2017, 529, 1600412.	0.9	4
237	Towards Time-Dependent Density-Functional Theory for Molecules in Strong Laser Pulses. Progress in Theoretical Chemistry and Physics, 2003, , 69-77.	0.2	4
238	42214 layered Fe-based superconductors: An <i>ab initio</i> study of their structural, magnetic, and electronic properties. Physical Review B, 2016, 93, .	1.1	3
239	Molecules and clusters in strong laser fields. , 2007, , 485-617.		3
240	Geometric energy transfer in two-component systems. Philosophical Transactions Series A, Mathematical, Physical, and Engineering Sciences, 2022, 380, 20200383.	1.6	3
241	Theory of relativistic effects in superconductors. Physica C: Superconductivity and Its Applications, 1999, 317-318, 508-510.	0.6	2
242	<i>Ab-initio</i> Computation of Superconducting Properties of Elemental Superconductors and MgB ₂ . Journal of Superconductivity and Novel Magnetism, 2005, 18, 649-652.	0.5	2
243	Back to the Ground-State: Electron Gas. Lecture Notes in Physics, 2006, , 423-434.	0.3	2
244	<i>Ab initio</i> study of doping effects in the 42214 compounds: A new family of layered iron-based superconductors. Physical Review B, 2017, 95, .	1.1	2
245	Direct evaluation of the isotope effect within the framework of density functional theory for superconductors. Journal of Physics Condensed Matter, 2019, 31, 334001.	0.7	2
246	Density Functional Theory of the Superconducting State. NATO ASI Series Series B: Physics, 1995, , 431-460.	0.2	2
247	Solution of the extended Thomas-Fermi model for triatomic molecules. Journal of Physics B: Atomic and Molecular Physics, 1981, 14, 2753-2759.	1.6	1
248	Optimal control of charge transfer. , 2006, 6325, 114.		1
249	Density functional theory for superconductors. International Journal of Quantum Chemistry, 1989, 36, 611-615.	1.0	1
250	Transport properties of chrysazine-type molecules. Theoretical Chemistry Accounts, 2010, 125, 535-541.	0.5	1
251	Virial theorem and exact properties of density functionals for periodic systems. Physical Review B, 2014, 89, .	1.1	1
252	Experimental and theoretical structural/spectroscopical correlation of enterobactin and catecholamide. Data in Brief, 2018, 20, 2054-2064.	0.5	1

#	ARTICLE	IF	CITATIONS
253	Orbital Functionals in Static and Time-Dependent Density Functional Theory. , 1999, , 393-427.		1
254	Rebuttal to the "Comment on Electromagnetic potential in Thomas-Fermi-Dirac atoms". Physical Review A, 1981, 23, 2087-2087.	1.0	0
255	Controlling observables in normal, hybrid and Josephson junctions. Molecular Physics, 2018, 116, 2449-2460.	0.8	0