Eberhard K U Gross

List of Publications by Year
in descending order

256	29,567	11651 70	4991 167
papers	citations	h-index	g-index

258	258	258	16904
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	Density-Functional Theory for Time-Dependent Systems. Physical Review Letters, 1984, 52, 997-1000.	7.8	7,180
2	Excitation Energies from Time-Dependent Density-Functional Theory. Physical Review Letters, 1996, 76, 1212-1215.	7.8	1,466
3	Reproducibility in density functional theory calculations of solids. Science, 2016, 351, aad3000.	12.6	1,113
4	TIME-DEPENDENT DENSITY FUNCTIONAL THEORY. Annual Review of Physical Chemistry, 2004, 55, 427-455.	10.8	1,099
5	Time-Dependent Density-Functional Theory. Advances in Quantum Chemistry, 1990, 21, 255-291.	0.8	992
6	Local density-functional theory of frequency-dependent linear response. Physical Review Letters, 1985, 55, 2850-2852.	7.8	939
7	Time-dependent density functional theory: Past, present, and future. Journal of Chemical Physics, 2005, 123, 062206.	3.0	791
8	octopus: a tool for the application of time-dependent density functional theory. Physica Status Solidi (B): Basic Research, 2006, 243, 2465-2488.	1.5	756
9	Density functional theory of time-dependent phenomena. , 1996, , 81-172.		476
10	Understanding band gaps of solids in generalized Kohnâ€“Sham theory. Proceedings of the National Academy of Sciences of the United States of America, 2017, 114, 2801-2806.	7.1	423
11	Fundamentals of Time-Dependent Density Functional Theory. Lecture Notes in Physics, 2012, , .	0.7	370
12	Exact Coulomb cutoff technique for supercell calculations. Physical Review B, 2006, 73, .	3.2	369
13	Density-Functional Theory for Superconductors. Physical Review Letters, 1988, 60, 2430-2433.	7.8	362
14	How to represent crystal structures for machine learning: Towards fast prediction of electronic properties. Physical Review B, 2014, 89, .	3.2	353
15	Exact Factorization of the Time-Dependent Electron-Nuclear Wave Function. Physical Review Letters, 2010, 105, 123002.	7.8	351
16	Quantum optimal control theory. Journal of Physics B: Atomic, Molecular and Optical Physics, 2007, 40, R175-R211.	1.5	330
17	Ab initiotheory of superconductivity. I. Density functional formalism and approximate functionals. Physical Review B, 2005, 72, .	3.2	314
18	Density-functional theory for ensembles of fractionally occupied states. I. Basic formalism. Physical Review A, 1988, 37, 2809-2820.	2.5	301

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19	Time-dependent quantum transport: A practical scheme using density functional theory. Physical Review B, 2005, 72, .	3.2	291
20	Rayleigh-Ritz variational principle for ensembles of fractionally occupied states. Physical Review A, 1988, 37, 2805-2808.	2.5	281
21	Intense-Field Double Ionization of Helium: Identifying the Mechanism. Physical Review Letters, 2000, 85, 4707-4710.	7.8	278
22	Ab initiotheory of superconductivity. II. Application to elemental metals. Physical Review B, 2005, 72, .	3.2	261
23	Density-functional theory for ensembles of fractionally occupied states. II. Application to the He atom. Physical Review A, 1988, 37, 2821-2833.	2.5	237
24	Time-Dependent Optimized Effective Potential. Physical Review Letters, 1995, 74, 872-875.	7.8	222
25	Multicomponent Density-Functional Theory for Electrons and Nuclei. Physical Review Letters, 2001, 86, 2984-2987.	7.8	206
26	AbÂInitioDescription of High-Temperature Superconductivity in Dense Molecular Hydrogen. Physical Review Letters, 2008, 100, 257001.	7.8	199
27	Correlated electron-nuclear dynamics: Exact factorization of the molecular wavefunction. Journal of Chemical Physics, 2012, 137, 22A530.	3.0	198
28	Laser-Induced Demagnetization at Ultrashort Time Scales: Predictions of TDDFT. Journal of Chemical Theory and Computation, 2015, 11, 4870-4874.	5.3	167
29	Bootstrap Approximation for the Exchange-Correlation Kernel of Time-Dependent Density-Functional Theory. Physical Review Letters, 2011, 107, 186401.	7.8	164
30	Superconductivity in Lithium, Potassium, and Aluminum under Extreme Pressure: A First-Principles Study. Physical Review Letters, 2006, 96, 047003.	7.8	159
31	Excitations in Time-Dependent Density-Functional Theory. Physical Review Letters, 2003, 90, 043005.	7.8	156
32	High temperature superconductivity in sulfur and selenium hydrides at high pressure. European Physical Journal B, 2016, 89, 1.	1.5	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.	7.8	141
34	Density-functional theory using an optimized exchange-correlation potential. Chemical Physics Letters, 1995, 240, 141-150.	2.6	140
35	Reduced density matrix functional for many-electron systems. Physical Review B, 2008, 78, .	3.2	138
36	Superconducting Properties ofMgB2from First Principles. Physical Review Letters, 2005, 94, 037004.	7.8	137

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37	Coupled-Trajectory Quantum-Classical Approach to Electronic Decoherence in Nonadiabatic Processes. Physical Review Letters, 2015, 115, 073001.	7.8	126
38	Adiabatic Approximation in Nonperturbative Time-Dependent Density-Functional Theory. Physical Review Letters, 2008, 100, 153004.	7.8	125
39	Superconductivity in metastable phases of phosphorus-hydride compounds under high pressure. Physical Review B, 2016, 93, .	3.2	125
40	Ab Initio Nonadiabatic Dynamics with Coupled Trajectories: A Rigorous Approach to Quantum (De)Coherence. Journal of Physical Chemistry Letters, 2017, 8, 3048-3055.	4.6	123
41	Time-dependent electron localization function. Physical Review A, 2005, 71, .	2.5	122
42	Quantum-Classical Nonadiabatic Dynamics: Coupled- vs Independent-Trajectory Methods. Journal of Chemical Theory and Computation, 2016, 12, 2127-2143.	5.3	117
43	Time-dependent approach to electron pumping in open quantum systems. Physical Review B, 2008, 77, .	3.2	115
44	Dynamical Coulomb Blockade and the Derivative Discontinuity of Time-Dependent Density Functional Theory. Physical Review Letters, 2010, 104, 236801.	7.8	115
45	Electron correlation energies from scaled exchange-correlation kernels: Importance of spatial versus temporal nonlocality. Physical Review B, 2000, 61, 13431-13437.	3.2	113
46	Toward the description of van der Waals interactions within density functional theory. Journal of Computational Chemistry, 1999, 20, 12-22.	3.3	106
47	Even-Harmonic Generation due to Beyond-Born-Oppenheimer Dynamics. Physical Review Letters, 2001, 87, 103901.	7.8	105
48	Optimal Control of Quantum Rings by Terahertz Laser Pulses. Physical Review Letters, 2007, 98, 157404.	7.8	102
49	Anisotropic gap of superconductingCaC6: A first-principles density functional calculation. Physical Review B, 2007, 75, .	3.2	101
50	Time-Dependent Density Functional Theory beyond Linear Response: An Exchange-Correlation Potential with Memory. Physical Review Letters, 1997, 79, 1905-1908.	7.8	99
51	Thermal conductivity in PbTe from first principles. Physical Review B, 2015, 91, .	3.2	98
52	Strong-field ionization dynamics of a modelH2molecule. Physical Review A, 2002, 65, .	2.5	97
53	Spurious Interactions, and Their Correction, in the Ensemble-Kohn-Sham Scheme for Excited States. Physical Review Letters, 2002, 88, 033003.	7.8	94
54	Dynamical Steps that Bridge Piecewise Adiabatic Shapes in the Exact Time-Dependent Potential Energy Surface. Physical Review Letters, 2013, 110, 263001.	7.8	94

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55	Is the Molecular Berry Phase an Artifact of the Born-Oppenheimer Approximation?. Physical Review Letters, 2014, 113, 263004.	7.8	93
56	Local Density-Functional Theory of Frequency-Dependent Linear Response. Physical Review Letters, 1986, 57, 923-923.	7.8	91
57	Density-matrix-power functional: Performance for finite systems and the homogeneous electron gas. Physical Review A, 2009, 79, .	2.5	91
58	The exact forces on classical nuclei in non-adiabatic charge transfer. Journal of Chemical Physics, 2015, 142, 084303.	3.0	83
59	Vibrational properties of MnO and NiO from DFT<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:mo>+</mml:mo><mml:mspace width="0.28em" /><mml:mi>U</mml:mi></mml:mrow></mml:math>-based density functional perturbation theory. Physical Review B, 2011, 84, .	3.2	82
60	Ab initioangle- and energy-resolved photoelectron spectroscopy with time-dependent density-functional theory. Physical Review A, 2012, 85, .	2.5	82
61	Electronic non-adiabatic states: towards a density functional theory beyond the Bornâ€“Oppenheimer approximation. Philosophical Transactions Series A, Mathematical, Physical, and Engineering Sciences, 2014, 372, 20130059.	3.4	80
62	The 2021 room-temperature superconductivity roadmap. Journal of Physics Condensed Matter, 2022, 34, 183002.	1.8	79
63	Discontinuities of the exchange-correlation kernel and charge-transfer excitations in time-dependent density-functional theory. Physical Review A, 2012, 85, .	2.5	77
64	Correlation effects on the third-frequency-moment sum rule of electron liquids. Physical Review B, 1987, 35, 3003-3004.	3.2	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.	7.8	74
67	Two-band superconductivity in Pb fromab initiocalculations. Physical Review B, 2007, 75, .	3.2	73
68	Exact Conditions in Finite-Temperature Density-Functional Theory. Physical Review Letters, 2011, 107, 163001.	7.8	73
69	Correlation potentials for molecular bond dissociation within the self-consistent random phase approximation. Journal of Chemical Physics, 2012, 136, 034106.	3.0	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.	7.8	72
71	Ab initio Eliashberg Theory: Making Genuine Predictions of Superconducting Features. Journal of the Physical Society of Japan, 2018, 87, 041012.	1.6	72
72	Multicomponent density-functional theory for electrons and nuclei. Physical Review A, 2008, 78, .	2.5	70

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73	Time-Dependent Density-Functional Theory for Superconductors. Physical Review Letters, 1994, 73, 2915-2918.	7.8	68
74	Exact-exchange density-functional calculations for noble-gas solids. Physical Review B, 2004, 69, .	3.2	68
75	Nuclear velocity perturbation theory for vibrational circular dichroism: An approach based on the exact factorization of the electron-nuclear wave function. Journal of Chemical Physics, 2015, 143, 074106.	3.0	67
76	Optimal control of time-dependent targets. Physical Review A, 2005, 71, .	2.5	66
77	Gradient expansion of the Coulomb exchange energy. Zeitschrift FÃ¼r Physik A, 1981, 302, 103-106.	1.4	65
78	Density Functional Theory of Time-Dependent Systems. NATO ASI Series Series B: Physics, 1995, , 149-171.	0.2	65
79	Spectral Density and Metal-Insulator Phase Transition in Mott Insulators within Reduced Density Matrix Functional Theory. Physical Review Letters, 2013, 110, 116403.	7.8	65
80	Comparative study of many-body perturbation theory and time-dependent density functional theory in the out-of-equilibrium Anderson model. Physical Review B, 2011, 84, .	3.2	61
81	Electron-phonon interaction and superconductivity in metallic molecular hydrogen. II. Superconductivity under pressure. Physical Review B, 2010, 81, .	3.2	60
82	Ultrafast laser induced local magnetization dynamics in Heusler compounds. Scientific Reports, 2016, 6, 38911.	3.3	60
83	Thomas-Fermi approach to diatomic systems. I. Solution of the Thomas-Fermi and Thomas-Fermi-Dirac-WeizsÃcker equations. Physical Review A, 1979, 20, 1798-1807.	2.5	59
84	The optimized effective potential method of density functional theory: Applications to atomic and molecular systems. International Journal of Quantum Chemistry, 1997, 64, 95-110.	2.0	57
85	Excitation energies from time-dependent density functional theory using exact and approximate potentials. International Journal of Quantum Chemistry, 2000, 80, 534-554.	2.0	57
86	Mixed quantum-classical dynamics from the exact decomposition of electron-nuclear motion. Europhysics Letters, 2014, 106, 33001.	2.0	57
87	Classical nuclear motion coupled to electronic non-adiabatic transitions. Journal of Chemical Physics, 2014, 141, 214101.	3.0	54
88	Molecular geometric phase from the exact electron-nuclear factorization. Physical Review A, 2016, 93, .	2.5	54
89	Large magnetocrystalline anisotropy in tetragonally distorted Heuslers: a systematic study. Journal Physics D: Applied Physics, 2017, 50, 095002.	2.8	52
90	Mixed quantum-classical dynamics on the exact time-dependent potential energy surface: a fresh look at non-adiabatic processes. Molecular Physics, 2013, 111, 3625-3640.	1.7	51

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91	Exact Factorization-Based Density Functional Theory of Electrons and Nuclei. Physical Review Letters, 2016, 117, 193001.	7.8	50
92	The optimal one dimensional periodic table: a modified Pettifor chemical scale from data mining. New Journal of Physics, 2016, 18, 093011.	2.9	50
93	Performance of one-body reduced density-matrix functionals for the homogeneous electron gas. Physical Review B, 2007, 75, .	3.2	49
94	Competing Spin Transfer and Dissipation at<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" 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">)</mm	7.8	48
95	Physical Review Letters, 2019, 122, 067202. Electron-phonon interaction and superconductivity in metallic molecular hydrogen. I. Electronic and dynamical properties under pressure. Physical Review B, 2010, 81, .	3.2	47
96	Transverse Spin-Gradient Functional for Noncollinear Spin-Density-Functional Theory. Physical Review Letters, 2013, 111, 156401.	7.8	47
97	Tailoring laser pulses with spectral and fluence constraints using optimal control theory. Journal of Optics B: Quantum and Semiclassical Optics, 2005, 7, S300-S312.	1.4	46
98	Superconducting properties of MgB2 from first principles. Physica C: Superconductivity and Its Applications, 2007, 456, 45-53.	1.2	46
99	Superconducting pairing mediated by spin fluctuations from first principles. Physical Review B, 2014, 90, .	3.2	46
100	Current density functional theory of spontaneously magnetised solids. Europhysics Letters, 1997, 40, 545-550.	2.0	44
101	Electronic Flux Density beyond the Bornâ€“Oppenheimer Approximation. Journal of Physical Chemistry A, 2016, 120, 3316-3325.	2.5	44
102	An efficient algorithm for time propagation as applied to linearized augmented plane wave method. Computer Physics Communications, 2016, 209, 92-95.	7.5	43
103	How Interatomic Steps in the Exact Kohnâ€“Sham Potential Relate to Derivative Discontinuities of the Energy. Journal of Physical Chemistry Letters, 2017, 8, 5974-5980.	4.6	43
104	Ultrafast demagnetization in bulk versus thin films: anab initiostudy. Journal of Physics Condensed Matter, 2017, 29, 224001.	1.8	42
105	Accurate solution of the Thomas-Fermi-Dirac-Weizsï¿½cker variational equations for the case of neutral atoms and positive ions. Zeitschrift FÃ¼r Physik A, 1982, 309, 5-11.	1.4	41
106	Scaling and virial theorems in current-density-functional theory. Physical Review A, 1996, 53, R5-R8.	2.5	41
107	Open shells in reduced-density-matrix-functional theory. Physical Review A, 2005, 72, .	2.5	41
108	Ab initioprediction of pressure-induced superconductivity in potassium. Physical Review B, 2006, 73, .	3.2	41

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109	Reversible Formation of 2D Electron Gas at the LaFeO₃/SrTiO₃ Interface via Control of Oxygen Vacancies. Advanced Materials, 2017, 29, 1604447.	21.0	41
110	Electronic SchrÃ¶dinger equation with nonclassical nuclei. Physical Review A, 2014, 89, .	2.5	40
111	Laser-induced electron localization in H₂⁺: mixed quantum-classical dynamics based on the exact time-dependent potential energy surface. Physical Chemistry Chemical Physics, 2015, 17, 29271-29280.	2.8	40
112	An exact factorization perspective on quantum interferences in nonadiabatic dynamics. Journal of Chemical Physics, 2016, 145, 034103.	3.0	40
113	Orbital magnetism in the density functional theory of superconductors. Journal De Physique, 1989, 50, 2601-2612.	1.8	40
114	Local Density Approximation for Superconductors. Physical Review Letters, 1999, 83, 2628-2631.	7.8	39
115	Electronic Structure via Potential Functional Approximations. Physical Review Letters, 2011, 106, 236404.	7.8	39
116	Exact Single-Electron Approach to the Dynamics of Molecules in Strong Laser Fields. Physical Review Letters, 2017, 118, 163202.	7.8	39
117	Time-dependent natural orbitals and occupation numbers. Europhysics Letters, 2010, 92, 23001.	2.0	38
118	Correlation effects in bistability at the nanoscale: Steady state and beyond. Physical Review B, 2012, 85, .	3.2	38
119	Time-dependent electron localization functions for coupled nuclear-electronic motion. Journal of Chemical Physics, 2004, 121, 9666-9670.	3.0	37
120	Discontinuity of the chemical potential in reduced-density-matrix-functional theory. Europhysics Letters, 2007, 77, 67003.	2.0	37
121	Local Measurement of the Eliashberg Function of Pb Islands: Enhancement of Electron-Phonon Coupling by Quantum Well States. Physical Review Letters, 2015, 114, 047002.	7.8	37
122	Bound states in time-dependent quantum transport: oscillations and memory effects in current and density. Physical Chemistry Chemical Physics, 2009, 11, 4535.	2.8	36
123	Response to â€œComment on â€˜Correlated electron-nuclear dynamics: Exact factorization of the molecular wavefunctionâ€• [J. Chem. Phys. 139, 087101 (2013)]. Journal of Chemical Physics, 2013, 139, 087102.	3.0	36
124	Discontinuities of the Chemical Potential in Reduced Density Matrix Functional Theory. Zeitschrift Fur Physikalische Chemie, 2010, 224, 467-480.	2.8	35
125	Ab initiotheory of iron-based superconductors. Physical Review B, 2016, 94, .	3.2	35
126	Ensemble-Density functional theory for excited states. International Journal of Quantum Chemistry, 1990, 38, 707-716.	2.0	34

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127	Relativistic framework for microscopic theories of superconductivity. I. The Dirac equation for superconductors. Physical Review B, 1999, 59, 7140-7154.	3.2	34
128	Exchange-energy functionals for finite two-dimensional systems. Physical Review B, 2007, 76, .	3.2	34
129	Femtosecond laser pulse shaping for enhanced ionization. Europhysics Letters, 2009, 87, 53001.	2.0	34
130	Enhancing and controlling single-atom high-harmonic generation spectra: a time-dependent density-functional scheme. European Physical Journal B, 2015, 88, 1.	1.5	34
131	Optimal control of laser-induced spinâ€“orbit mediated ultrafast demagnetization. New Journal of Physics, 2016, 18, 013014.	2.9	34
132	Multicomponent density-functional theory for time-dependent systems. Physical Review A, 2007, 76, .	2.5	33
133	On the mechanism of strong-field double photoionization in the helium atom. Journal of Physics B: Atomic, Molecular and Optical Physics, 2000, 33, 433-442.	1.5	32
134	Optimal laser control of double quantum dots. Physical Review B, 2008, 77, .	3.2	32
135	Electronic, vibrational, and superconducting properties of<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:mrow><mml:mtext>CaBeSi</mml:mtext></mml:mrow></mml:mrow></mml:math>: First-principles calculations. Physical Review B, 2009, 79, .	3.2	32
136	A functional of the one-body-reduced density matrix derived from the homogeneous electron gas: Performance for finite systems. Journal of Chemical Physics, 2009, 130, 064109.	3.0	32
137	The role of Coulomb interaction in the superconducting properties of CaC₆and H under pressure. Superconductor Science and Technology, 2009, 22, 034006.	3.5	32
138	Time-dependent density-functional and reduced density-matrix methods for few electrons: Exact versus adiabatic approximations. Chemical Physics, 2011, 391, 1-10.	1.9	32
139	Semiclassical analysis of the electronâ€nuclear coupling in electronic nonâ€adiabatic processes. Annalen Der Physik, 2015, 527, 546-555.	2.4	32
140	Spin-multiplet energies from time-dependent density functional theory. International Journal of Quantum Chemistry, 1996, 60, 1393-1401.	2.0	29
141	Asymptotic Properties of the Optimized Effective Potential. Advances in Quantum Chemistry, 1998, , 31-48.	0.8	29
142	Resonant inelastic soft x-ray scattering of Be chalcogenides. Physical Review B, 2006, 73, .	3.2	29
143	The role of bound states in time-dependent quantum transport. Applied Physics A: Materials Science and Processing, 2008, 93, 355-364.	2.3	29
144	Phononic self-energy effects and superconductivity in CaC<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:msub><mml:mrow /><mml:mn>6</mml:mn></mml:msub></mml:math>. Physical Review B, 2012, 85, .	3.2	29

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145	Paramagnons in FeSe close to a magnetic quantum phase transition:Ab initiostudy. Physical Review B, 2012, 86, .	3.2	29
146	Reduced-density-matrix-functional theory at finite temperature: Theoretical foundations. Physical Review A, 2015, 92, .	2.5	29
147	Optimization schemes for selective molecular cleavage with tailored ultrashort laser pulses. Chemical Physics, 2011, 391, 50-61.	1.9	28
148	Discrete peaks in above-threshold double-ionization spectra. Physical Review A, 2001, 64, .	2.5	27
149	Gaussian approximations for the exchange-energy functional of current-carrying states: Applications to two-dimensional systems. Physical Review A, 2009, 80, .	2.5	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, .	3.2	26
152	Correlation energy of finite two-dimensional systems: Toward nonempirical and universal modeling. Physical Review B, 2009, 79, .	3.2	26
153	Magnon spectrum of transition-metal oxides: Calculations including long-range magnetic interactions using the<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:mi>LSDA</mml:mi><mml:mo>+</mml:mo><mml:mi>U</mml:mi></mml:mrow></mml:math>meth Physical Review B, 2011, 84, .	3.2	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.	7.8	26
155	On the Mass of Atoms in Molecules: Beyond the Born-Oppenheimer Approximation. Physical Review X, 2017, 7, .	8.9	26
156	Thomas-Fermi approach to diatomic systems. II. Correlation diagrams for N-N and Ne-Ne. Physical Review A, 1979, 20, 1808-1815.	2.5	25
157	Potential functionals versus density functionals. Physical Review A, 2013, 88, .	2.5	25
158	Ensemble-Hartreeâ€“Fock scheme for excited states. The optimized effective potential method. Physica B: Condensed Matter, 2002, 318, 328-332.	2.7	24
159	Time-dependent variational approach to molecules in strong laser fields. Chemical Physics, 2004, 304, 183-202.	1.9	24
160	Optimized effective potential method in current-spin-density-functional theory. Physical Review A, 2006, 74, .	2.5	24
161	Discontinuous functional for linear-response time-dependent density-functional theory: The exact-exchange kernel and approximate forms. Physical Review A, 2013, 88, .	2.5	24
162	Ab initiotheory of superconductivity in a magnetic field. I. Spin density functional theory for superconductors and Eliashberg equations. Physical Review B, 2015, 92, .	3.2	24

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163	Electronic exchange in quantum rings: Beyond the local-density approximation. Physical Review B, 2009, 79, .	3.2	23
164	Source-Free Exchange-Correlation Magnetic Fields in Density Functional Theory. Journal of Chemical Theory and Computation, 2018, 14, 1247-1253.	5.3	23
165	Exchange-correlation orbital functionals in current-density functional theory: Application to a quantum dot in magnetic fields. Physical Review B, 2008, 77, .	3.2	22
166	Optimal control of strong-field ionization with time-dependent density-functional theory. Physical Review A, 2013, 88, .	2.5	22
167	Asymptotic analysis of the Berry curvature in the<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mrow><mml:mi>E</mml:mi><mml:mo>âŠ—</mml:mo><mml:mi>e</mml:mi> model. Physical Review A, 2017, 96, .	2.5	22
168	Density functional theory of electron transfer beyond the Born-Oppenheimer approximation: Case study of LiF. Journal of Chemical Physics, 2018, 148, 084110.	3.0	22
169	Relativistic theory of superconductivity. Physics Letters, Section A: General, Atomic and Solid State Physics, 1995, 198, 261-266.	2.1	21
170	Chapter 10 Time-dependent transport phenomena. Theoretical and Computational Chemistry, 2007, 17, 247-284.	0.4	21
171	Discontinuity of the chemical potential in reduced-density-matrix-functional theory for open-shell systems. Physical Review A, 2009, 79, .	2.5	21
172	Optical Response of Extended Systems Using Time-Dependent Density Functional Theory. Topics in Current Chemistry, 2014, 347, 235-257.	4.0	21
173	Multiplicity of solutions to<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mrow><mml:mi>G</mml:mi><mml:mi>W</mml:mi> approximations. Physical Review B, 2015, 92, .	3.2	21
174	Electron-nuclear wave-packet dynamics through a conical intersection. Journal of Chemical Physics, 2017, 146, 074304.	3.0	21
175	Surface hopping in laser-driven molecular dynamics. Physical Review A, 2017, 95, .	2.5	21
176	Density-functional theory of the superconducting state. International Journal of Quantum Chemistry, 1991, 40, 289-297.	2.0	20
177	Conventional Quantum Chemical Correlation Energy Versus Density-Functional Correlation Energy. ACS Symposium Series, 1996, , 42-53.	0.5	20
178	Approximate relativistic optimized potential method. Physical Review A, 1998, 57, 138-148.	2.5	20
179	Relativistic framework for microscopic theories of superconductivity. II. The Pauli equation for superconductors. Physical Review B, 1999, 59, 7155-7165.	3.2	20
180	Theory of Dichroism in the Electromagnetic Response of Superconductors. Physical Review Letters, 1997, 78, 3753-3756.	7.8	18

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181	Theoretical investigation of optical conductivity in Ba(Fe1â^'xCox)2As2. Physical Review B, 2011, 83, .	3.2	18
182	Ab initiotheory of superconductivity in a magnetic field. II. Numerical solution. Physical Review B, 2015, 92, .	3.2	18
183	Adiabatic Connection and the Kohnâ^'Sham Variety of Potentialâ^'Functional Theory. Journal of Chemical Theory and Computation, 2009, 5, 844-849.	5.3	17
184	Enhanced excitonic effects in the energy loss spectra of LiF and Ar at large momentum transfer. New Journal of Physics, 2012, 14, 053052.	2.9	17
185	Spectrum for Nonmagnetic Mott Insulators from Power Functional within Reduced Density Matrix Functional Theory. Journal of Chemical Theory and Computation, 2015, 11, 4895-4899.	5.3	17
186	Exact factorization-based density functional theory of electron-phonon systems. Physical Review B, 2019, 99, .	3.2	17
187	Phase-space analysis of double ionization. Optics Express, 2001, 8, 411.	3.4	16
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