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	The 2021 room-temperature superconductivity roadmap. Journal of Physics Condensed Matter, 2022, 34, 183002.	1.8	79
2	Energy, Momentum, and Angular Momentum Transfer between Electrons and Nuclei. Physical Review Letters, 2022, 128, 113001.	7.8	12
3	Geometric energy transfer in two-component systems. Philosophical Transactions Series A, Mathematical, Physical, and Engineering Sciences, 2022, 380, 20200383.	3.4	3
4	Fock-Space Embedding Theory: Application to Strongly Correlated Topological Phases. Physical Review Letters, 2021, 127, 116401.	7.8	8
5	Many-body Green's function theory of electrons and nuclei beyond the Born-Oppenheimer approximation. Physical Review B, 2020, 101, .	3.2	10
6	Generation of magnetic skyrmions by focused vortex laser pulses. Journal of Applied Physics, 2020, 127, .	2.5	13
7	Complete description of the magnetic ground state in spinel vanadates. Physical Review B, 2019, 100, .	3.2	7
8	Electron-nuclear entanglement in the time-dependent molecular wavefunction. Computational and Theoretical Chemistry, 2019, 1151, 99-106.	2.5	14
9	Direct evaluation of the isotope effect within the framework of density functional theory for superconductors. Journal of Physics Condensed Matter, 2019, 31, 334001.	1.8	2
10	Exact factorization-based density functional theory of electron-phonon systems. Physical Review B, 2019, 99, .	3.2	17
11	Model Hamiltonian for strongly correlated systems: Systematic, self-consistent, and unique construction. Physical Review B, 2019, 99, .	3.2	8
12	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 50 292 Td (stretchy="false">)</mml:mo></mml:mrow></mml:math>Interfaces. Physical Review Letters, 2019, 122, 067202.	7.8	48
13	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
14	IR and NMR spectroscopic correlation of enterobactin by DFT. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2018, 198, 264-277.	3.9	10
15	Ab initio Eliashberg Theory: Making Genuine Predictions of Superconducting Features. Journal of the Physical Society of Japan, 2018, 87, 041012.	1.6	72
16	Source-Free Exchange-Correlation Magnetic Fields in Density Functional Theory. Journal of Chemical Theory and Computation, 2018, 14, 1247-1253.	5.3	23
17	Controlling observables in normal, hybrid and Josephson junctions. Molecular Physics, 2018, 116, 2449-2460.	1.7	0
18	Accurate Formula for the Macroscopic Polarization of Strongly Correlated Materials. Journal of Physical Chemistry Letters, 2018, 9, 7045-7051.	4.6	8

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19	Experimental and theoretical structural/spectroscopical correlation of enterobactin and catecholamide. Data in Brief, 2018, 20, 2054-2064.	1.0	1
20	Ab initiostudy of doping effects in the 42214 compounds: A new family of layered iron-based superconductors. Physical Review B, 2017, 95, .	3.2	2
21	Reversible Formation of 2D Electron Gas at the LaFeO₃/SrTiO₃ Interface via Control of Oxygen Vacancies. Advanced Materials, 2017, 29, 1604447.	21.0	41
22	Electron-nuclear wave-packet dynamics through a conical intersection. Journal of Chemical Physics, 2017, 146, 074304.	3.0	21
23	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
24	Ultrafast demagnetization in bulk versus thin films: anab initiostudy. Journal of Physics Condensed Matter, 2017, 29, 224001.	1.8	42
25	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
26	On the Mass of Atoms in Molecules: Beyond the Born-Oppenheimer Approximation. Physical Review X, 2017, 7, .	8.9	26
27	L1₀ Stacked Binaries as Candidates for Hardâ€Magnets: FePt, MnAl and MnGa. Annalen Der Physik, 2017, 529, 1600412.	2.4	4
28	Large magnetocrystalline anisotropy in tetragonally distorted Heuslers: a systematic study. Journal Physics D: Applied Physics, 2017, 50, 095002.	2.8	52
29	Exact Single-Electron Approach to the Dynamics of Molecules in Strong Laser Fields. Physical Review Letters, 2017, 118, 163202.	7.8	39
30	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
31	Spin-density fluctuations and the fluctuation-dissipation theorem in <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mrow><mml:mn>3</mml:mn><mml:mi>d</mml:mi></mml:mrow></mml:math> ferromagnetic metals. Physical Review B, 2017, 96, .	3.2	12
32	Surface hopping in laser-driven molecular dynamics. Physical Review A, 2017, 95, .	2.5	21
33	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:mrow></mml:math>e model. Physical Review A, 2017, 96, .	2.5	12
34	Exchange-correlation approximations for reduced-density-matrix-functional theory at finite temperature: Capturing magnetic phase transitions in the homogeneous electron gas. Physical Review A, 2017, 96, .	2.5	7
35	Optimal control of laser-induced spinâ€“orbit mediated ultrafast demagnetization. New Journal of Physics, 2016, 18, 013014.	2.9	34
36	An exact factorization perspective on quantum interferences in nonadiabatic dynamics. Journal of Chemical Physics, 2016, 145, 034103.	3.0	40

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37	Quantum-Classical Nonadiabatic Dynamics: Coupled- vs Independent-Trajectory Methods. Journal of Chemical Theory and Computation, 2016, 12, 2127-2143.	5.3	117
38	An efficient algorithm for time propagation as applied to linearized augmented plane wave method. Computer Physics Communications, 2016, 209, 92-95.	7.5	43
39	Comment on â€œEstimating Excitonic Effects in the Absorption Spectra of Solids: Problems and Insight from a Guided Iteration Schemeâ€. Physical Review Letters, 2016, 117, 159701.	7.8	6
40	Molecular geometric phase from the exact electron-nuclear factorization. Physical Review A, 2016, 93, .	2.5	54
41	Superconductivity in metastable phases of phosphorus-hydride compounds under high pressure. Physical Review B, 2016, 93, .	3.2	125
42	42214 layered Fe-based superconductors: Anab initiostudy of their structural, magnetic, and electronic properties. Physical Review B, 2016, 93, .	3.2	3
43	Ab initiotheory of iron-based superconductors. Physical Review B, 2016, 94, .	3.2	35
44	Exact Factorization-Based Density Functional Theory of Electrons and Nuclei. Physical Review Letters, 2016, 117, 193001.	7.8	50
45	The optimal one dimensional periodic table: a modified Pettifor chemical scale from data mining. New Journal of Physics, 2016, 18, 093011.	2.9	50
46	Swift thermal steering of domain walls in ferromagnetic MnBi stripes. Scientific Reports, 2016, 6, 24411.	3.3	10
47	Ultrafast laser induced local magnetization dynamics in Heusler compounds. Scientific Reports, 2016, 6, 38911.	3.3	60
48	High temperature superconductivity in sulfur and selenium hydrides at high pressure. European Physical Journal B, 2016, 89, 1.	1.5	154
49	Reproducibility in density functional theory calculations of solids. Science, 2016, 351, aad3000.	12.6	1,113
50	Electronic Flux Density beyond the Bornâ€“Oppenheimer Approximation. Journal of Physical Chemistry A, 2016, 120, 3316-3325.	2.5	44
51	Almost exact exchange at almost no computational cost in electronic structure. Physical Review A, 2015, 92, .	2.5	11
52	Reduced-density-matrix-functional theory at finite temperature: Theoretical foundations. Physical Review A, 2015, 92, .	2.5	29
53	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></mml:mrow></mml approximations. Physical Review B, 2015, 92, .	3.2	21
54	Coupled-Trajectory Quantum-Classical Approach to Electronic Decoherence in Nonadiabatic Processes. Physical Review Letters, 2015, 115, 073001.	7.8	126

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55	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
56	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
57	Doping induced metal-insulator phase transition in NiOâ€”a reduced density matrix functional theory perspective. New Journal of Physics, 2015, 17, 093038.	2.9	10
58	Semiclassical analysis of the electronâ€•nuclear coupling in electronic nonâ€•adiabatic processes. Annalen Der Physik, 2015, 527, 546-555.	2.4	32
59	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
60	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
61	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
62	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
63	The exact forces on classical nuclei in non-adiabatic charge transfer. Journal of Chemical Physics, 2015, 142, 084303.	3.0	83
64	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
65	Ab initiotheory of superconductivity in a magnetic field. II. Numerical solution. Physical Review B, 2015, 92, .	3.2	18
66	Thermal conductivity in PbTe from first principles. Physical Review B, 2015, 91, .	3.2	98
67	Excitons in Organics Using Time-Dependent Density Functional Theory: PPV, Pentacene, and Picene. Journal of Chemical Theory and Computation, 2015, 11, 1710-1714.	5.3	13
68	Laser-Induced Demagnetization at Ultrashort Time Scales: Predictions of TDDFT. Journal of Chemical Theory and Computation, 2015, 11, 4870-4874.	5.3	167
69	Is the Molecular Berry Phase an Artifact of the Born-Oppenheimer Approximation?. Physical Review Letters, 2014, 113, 263004.	7.8	93
70	Classical nuclear motion coupled to electronic non-adiabatic transitions. Journal of Chemical Physics, 2014, 141, 214101.	3.0	54
71	Superconducting pairing mediated by spin fluctuations from first principles. Physical Review B, 2014, 90, .	3.2	46
72	Electronic SchrÃ¶dinger equation with nonclassical nuclei. Physical Review A, 2014, 89, .	2.5	40

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73	How to represent crystal structures for machine learning: Towards fast prediction of electronic properties. Physical Review B, 2014, 89, .	3.2	353
74	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
75	Optimal control theory for quantum-classical systems: Ehrenfest molecular dynamics based on time-dependent density-functional theory. Journal of Physics A: Mathematical and Theoretical, 2014, 47, 025204.	2.1	11
76	Optical Response of Extended Systems Using Time-Dependent Density Functional Theory. Topics in Current Chemistry, 2014, 347, 235-257.	4.0	21
77	Mixed quantum-classical dynamics from the exact decomposition of electron-nuclear motion. Europhysics Letters, 2014, 106, 33001.	2.0	57
78	Virial theorem and exact properties of density functionals for periodic systems. Physical Review B, 2014, 89, .	3.2	1
79	Potential functionals versus density functionals. Physical Review A, 2013, 88, .	2.5	25
80	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
81	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
82	Minimization procedure in reduced density matrix functional theory by means of an effective noninteracting system. Computational and Theoretical Chemistry, 2013, 1003, 114-122.	2.5	14
83	Dynamical Steps that Bridge Piecewise Adiabatic Shapes in the Exact Time-Dependent Potential Energy Surface. Physical Review Letters, 2013, 110, 263001.	7.8	94
84	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
85	Transverse Spin-Gradient Functional for Noncollinear Spin-Density-Functional Theory. Physical Review Letters, 2013, 111, 156401.	7.8	47
86	Optimal control of strong-field ionization with time-dependent density-functional theory. Physical Review A, 2013, 88, .	2.5	22
87	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
88	Effect of discontinuities in Kohn-Sham-based chemical reactivity theory. Journal of Chemical Physics, 2012, 136, 114102.	3.0	13
89	Correlation potentials for molecular bond dissociation within the self-consistent random phase approximation. Journal of Chemical Physics, 2012, 136, 034106.	3.0	72
90	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

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91	Discontinuities of the exchange-correlation kernel and charge-transfer excitations in time-dependent density-functional theory. Physical Review A, 2012, 85, .	2.5	77
92	Correlation effects in bistability at the nanoscale: Steady state and beyond. Physical Review B, 2012, 85, .	3.2	38
93	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
94	First-principles study of rare-earth-doped superconducting CaFe<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:msub><mml:mrow /><mml:mn>2</mml:mn></mml:msub></mml:math>As<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:msub><mml:mrow /><mml:mn>2</mml:mn></mml:msub></mml:math>. Physical Review B, 2012, 86, .	3.2	15
95	Ab initioangle- and energy-resolved photoelectron spectroscopy with time-dependent density-functional theory. Physical Review A, 2012, 85, .	2.5	82
96	Paramagnons in FeSe close to a magnetic quantum phase transition:Ab initiostudy. Physical Review B, 2012, 86, .	3.2	29
97	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
98	Correlated electron-nuclear dynamics: Exact factorization of the molecular wavefunction. Journal of Chemical Physics, 2012, 137, 22A530.	3.0	198
99	Ionization potentials and electron affinities from reduced-density-matrix functional theory. Physical Review A, 2012, 85, .	2.5	15
100	Fundamentals of Time-Dependent Density Functional Theory. Lecture Notes in Physics, 2012, , .	0.7	370
101	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
102	Bootstrap Approximation for the Exchange-Correlation Kernel of Time-Dependent Density-Functional Theory. Physical Review Letters, 2011, 107, 186401.	7.8	164
103	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
104	Exact Conditions in Finite-Temperature Density-Functional Theory. Physical Review Letters, 2011, 107, 163001.	7.8	73
105	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
106	Optimization schemes for selective molecular cleavage with tailored ultrashort laser pulses. Chemical Physics, 2011, 391, 50-61.	1.9	28
107	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
108	Electronic Structure via Potential Functional Approximations. Physical Review Letters, 2011, 106, 236404.	7.8	39

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109	Theoretical investigation of optical conductivity in Ba(Fe1â^'xCox)2As2. Physical Review B, 2011, 83, .	3.2	18
110	Discontinuities of the Chemical Potential in Reduced Density Matrix Functional Theory. Zeitschrift Fur Physikalische Chemie, 2010, 224, 467-480.	2.8	35
111	Transport properties of chrysazine-type molecules. Theoretical Chemistry Accounts, 2010, 125, 535-541.	1.4	1
112	Electron-phonon interaction and superconductivity in metallic molecular hydrogen. I. Electronic and dynamical properties under pressure. Physical Review B, 2010, 81, .	3.2	47
113	Noncollinear spin-spiral phase for the uniform electron gas within reduced-density-matrix-functional theory. Physical Review B, 2010, 81, .	3.2	9
114	Static and dynamical susceptibility ofLaO1â^'xFxFeAs. Physical Review B, 2010, 81, .	3.2	6
115	Time-dependent natural orbitals and occupation numbers. Europhysics Letters, 2010, 92, 23001.	2.0	38
116	Dynamical Coulomb Blockade and the Derivative Discontinuity of Time-Dependent Density Functional Theory. Physical Review Letters, 2010, 104, 236801.	7.8	115
117	Exact Factorization of the Time-Dependent Electron-Nuclear Wave Function. Physical Review Letters, 2010, 105, 123002.	7.8	351
118	Electron-phonon interaction and superconductivity in metallic molecular hydrogen. II. Superconductivity under pressure. Physical Review B, 2010, 81, .	3.2	60
119	Acceleration of quantum optimal control theory algorithms with mixing strategies. Physical Review E, 2009, 79, 056704.	2.1	10
120	Magnetism in<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:msub><mml:mrow><mml:mtext>CeFeAsO</mml:mtext></mml:mrow><mml:mrow><mml:mn>1</m xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:msub><mml:mrow><mml:mtext>LaFeAsO</mml:mtext></mml:mrow><mml:mrow><mml:mn>1</m Physical Review B, 2009, 80, .	3.2	14
121	Discontinuity of the chemical potential in reduced-density-matrix-functional theory for open-shell systems. Physical Review A, 2009, 79, .	2.5	21
122	Electronic exchange in quantum rings: Beyond the local-density approximation. Physical Review B, 2009, 79, .	3.2	23
123	Gaussian approximations for the exchange-energy functional of current-carrying states: Applications to two-dimensional systems. Physical Review A, 2009, 80, .	2.5	27
124	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
125	Correlation energy of finite two-dimensional systems: Toward nonempirical and universal modeling. Physical Review B, 2009, 79, .	3.2	26
126	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

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127	Multiband superconductivity in Pb, H under pressure and CaBeSi fromab initiocalculations. Journal of Physics Condensed Matter, 2009, 21, 164209.	1.8	10
128	Adiabatic Connection and the Kohnâ"Sham Variety of Potentialâ"Functional Theory. Journal of Chemical Theory and Computation, 2009, 5, 844-849.	5.3	17
129	Femtosecond laser pulse shaping for enhanced ionization. Europhysics Letters, 2009, 87, 53001.	2.0	34
130	The role of Coulomb interaction in the superconducting properties of CaC₆and H under pressure. Superconductor Science and Technology, 2009, 22, 034006.	3.5	32
131	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
132	Density-matrix-power functional: Performance for finite systems and the homogeneous electron gas. Physical Review A, 2009, 79, .	2.5	91
133	The role of bound states in time-dependent quantum transport. Applied Physics A: Materials Science and Processing, 2008, 93, 355-364.	2.3	29
134	Coherent quantum switch driven by optimized laser pulses. Physica E: Low-Dimensional Systems and Nanostructures, 2008, 40, 1593-1595.	2.7	6
135	Adiabatic Approximation in Nonperturbative Time-Dependent Density-Functional Theory. Physical Review Letters, 2008, 100, 153004.	7.8	125
136	Reduced density matrix functional for many-electron systems. Physical Review B, 2008, 78, .	3.2	138
137	Electron localization function for two-dimensional systems. Physical Review B, 2008, 77, .	3.2	16
138	Time-dependent approach to electron pumping in open quantum systems. Physical Review B, 2008, 77, .	3.2	115
139	Optimal laser control of double quantum dots. Physical Review B, 2008, 77, .	3.2	32
140	AbÂInitioDescription of High-Temperature Superconductivity in Dense Molecular Hydrogen. Physical Review Letters, 2008, 100, 257001.	7.8	199
141	Publisherâ€™s Note:Ab initioDescription of High-Temperature Superconductivity in Dense Molecular Hydrogen [Phys. Rev. Lett.100, 257001 (2008)]. Physical Review Letters, 2008, 101, .	7.8	4
142	Multicomponent density-functional theory for electrons and nuclei. Physical Review A, 2008, 78, .	2.5	70
143	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
144	Orbital currents in the Colle-Salvetti correlation energy functional and the degeneracy problem. Journal of Chemical Physics, 2007, 127, 124103.	3.0	11

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145	Two-band superconductivity in Pb fromab initiocalculations. Physical Review B, 2007, 75, .	3.2	73
146	Multicomponent density-functional theory for time-dependent systems. Physical Review A, 2007, 76, .	2.5	33
147	Comparison of exact-exchange calculations for solids in current-spin-density- and spin-density-functional theory. Physical Review B, 2007, 76, .	3.2	26
148	First-Principles Approach to Noncollinear Magnetism: Towards Spin Dynamics. Physical Review Letters, 2007, 98, 196405.	7.8	74
149	Performance of one-body reduced density-matrix functionals for the homogeneous electron gas. Physical Review B, 2007, 75, .	3.2	49
150	Exchange-energy functionals for finite two-dimensional systems. Physical Review B, 2007, 76, .	3.2	34
151	Optimal Control of Quantum Rings by Terahertz Laser Pulses. Physical Review Letters, 2007, 98, 157404.	7.8	102
152	Chapter 10 Time-dependent transport phenomena. Theoretical and Computational Chemistry, 2007, 17, 247-284.	0.4	21
153	Discontinuity of the chemical potential in reduced-density-matrix-functional theory. Europhysics Letters, 2007, 77, 67003.	2.0	37
154	Quantum optimal control theory. Journal of Physics B: Atomic, Molecular and Optical Physics, 2007, 40, R175-R211.	1.5	330
155	Anisotropic gap of superconductingCaC6: A first-principles density functional calculation. Physical Review B, 2007, 75, .	3.2	101
156	XMCD Analysis Beyond Standard Procedures. AIP Conference Proceedings, 2007, , .	0.4	10
157	Superconducting properties of MgB2 from first principles. Physica C: Superconductivity and Its Applications, 2007, 456, 45-53.	1.2	46
158	Molecules and clusters in strong laser fields. , 2007, , 485-617.		3
159	Ab initioprediction of pressure-induced superconductivity in potassium. Physical Review B, 2006, 73, .	3.2	41
160	Exact Coulomb cutoff technique for supercell calculations. Physical Review B, 2006, 73, .	3.2	369
161	Optimal control of charge transfer. , 2006, 6325, 114.		1
162	Double-pole approximation in time-dependent density functional theory. International Journal of Quantum Chemistry, 2006, 106, 2840-2847.	2.0	6

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163	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
164	On the degeneracy of atomic states within exact-exchange (spin-) density functional theory. Journal of Chemical Physics, 2006, 125, 084105.	3.0	13
165	Back to the Ground-State: Electron Gas. Lecture Notes in Physics, 2006, , 423-434.	0.7	2
166	Optimized effective potential method in current-spin-density-functional theory. Physical Review A, 2006, 74, .	2.5	24
167	Superconductivity in Lithium, Potassium, and Aluminum under Extreme Pressure: A First-Principles Study. Physical Review Letters, 2006, 96, 047003.	7.8	159
168	Resonant inelastic soft x-ray scattering of Be chalcogenides. Physical Review B, 2006, 73, .	3.2	29
169	Ab-initio Computation of Superconducting Properties of Elemental Superconductors and MgB2. Journal of Superconductivity and Novel Magnetism, 2005, 18, 649-652.	0.5	2
170	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
171	Time-dependent electron localization function. Physical Review A, 2005, 71, .	2.5	122
172	Superconducting Properties ofMgB2from First Principles. Physical Review Letters, 2005, 94, 037004.	7.8	137
173	Measuring the Kernel of Time-Dependent Density Functional Theory with X-Ray Absorption Spectroscopy of3dTransition Metals. Physical Review Letters, 2005, 95, 253006.	7.8	16
174	Open shells in reduced-density-matrix-functional theory. Physical Review A, 2005, 72, .	2.5	41
175	Optimal control of time-dependent targets. Physical Review A, 2005, 71, .	2.5	66
176	Ab initiotheory of superconductivity. II. Application to elemental metals. Physical Review B, 2005, 72, .	3.2	261
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