Eberhard K U Gross

List of Publications by Citations

256 papers	25,012 citations	65 h-index	155 g-index
257 ext. papers	27,276 ext. citations	4.1 avg, IF	7.06 L-index

#	Paper	IF	Citations
256	Density-Functional Theory for Time-Dependent Systems. *Physical Review Letters*, **1984**, 52, 997-1000	7.4	6170
255	Excitation energies from time-dependent density-functional theory. *Physical Review Letters*, **1996**, 76, 1212-1215	7.4	1324
254	Time-dependent density functional theory. *Annual Review of Physical Chemistry*, **2004**, 55, 427-55	15.7	932
253	Time-Dependent Density-Functional Theory. *Advances in Quantum Chemistry*, **1990**, 21, 255-291	1.4	893
252	Local density-functional theory of frequency-dependent linear response. *Physical Review Letters*, **1985**, 55, 2850-2852	7.4	832
251	Reproducibility in density functional theory calculations of solids. *Science*, **2016**, 351, aad3000	33.3	784
250	Time-dependent density functional theory: past, present, and future. *Journal of Chemical Physics*, **2005**, 123, 62206	3.9	665
249	octopus: a tool for the application of time-dependent density functional theory. *Physica Status Solidi (B): Basic Research*, **2006**, 243, 2465-2488	1.3	659
248	Density functional theory of time-dependent phenomena **1996**, 81-172		424
247	Exact Coulomb cutoff technique for supercell calculations. *Physical Review B*, **2006**, 73,	3.3	286
246	Exact factorization of the time-dependent electron-nuclear wave function. *Physical Review Letters*, **2010**, 105, 123002	7.4	285
245	Density-functional theory for superconductors. *Physical Review Letters*, **1988**, 60, 2430-2433	7.4	281
244	Understanding band gaps of solids in generalized Kohn-Sham theory. *Proceedings of the National Academy of Sciences of the United States of America*, **2017**, 114, 2801-2806	11.5	280
243	Fundamentals of Time-Dependent Density Functional Theory. *Lecture Notes in Physics*, **2012**,	0.8	277
242	How to represent crystal structures for machine learning: Towards fast prediction of electronic properties. *Physical Review B*, **2014**, 89,	3.3	275
241	Time-dependent quantum transport: A practical scheme using density functional theory. *Physical Review B*, **2005**, 72,	3.3	275
240	Density-functional theory for ensembles of fractionally occupied states. I. Basic formalism. *Physical Review A*, **1988**, 37, 2809-2820	2.6	271

239	Quantum optimal control theory. *Journal of Physics B: Atomic, Molecular and Optical Physics*, **2007**, 40, R175-R211	1.3	258
238	Intense-field double ionization of helium: identifying the mechanism. *Physical Review Letters*, **2000**, 85, 4707-10	7.4	255
237	Rayleigh-Ritz variational principle for ensembles of fractionally occupied states. *Physical Review A*, **1988**, 37, 2805-2808	2.6	252
236	Ab initio theory of superconductivity. I. Density functional formalism and approximate functionals. *Physical Review B*, **2005**, 72,	3.3	237
235	Density-functional theory for ensembles of fractionally occupied states. II. Application to the He atom. *Physical Review A*, **1988**, 37, 2821-2833	2.6	222
234	Time-dependent optimized effective potential. *Physical Review Letters*, **1995**, 74, 872-875	7.4	211
233	Ab initio theory of superconductivity. II. Application to elemental metals. *Physical Review B*, **2005**, 72,	3.3	199
232	Multicomponent density-functional theory for electrons and nuclei. *Physical Review Letters*, **2001**, 86, 2984-7	7.4	183
231	Ab initio description of high-temperature superconductivity in dense molecular hydrogen. *Physical Review Letters*, **2008**, 100, 257001	7.4	167
230	Correlated electron-nuclear dynamics: exact factorization of the molecular wavefunction. *Journal of Chemical Physics*, **2012**, 137, 22A530	3.9	157
229	Excitations in time-dependent density-functional theory. *Physical Review Letters*, **2003**, 90, 043005	7.4	148
228	Superconductivity in lithium, potassium, and aluminum under extreme pressure: a first-principles study. *Physical Review Letters*, **2006**, 96, 047003	7.4	138
227	Density-functional theory using an optimized exchange-correlation potential. *Chemical Physics Letters*, **1995**, 240, 141-150	2.5	137
226	Bootstrap approximation for the exchange-correlation kernel of time-dependent density-functional theory. *Physical Review Letters*, **2011**, 107, 186401	7.4	131
225	High temperature superconductivity in sulfur and selenium hydrides at high pressure. *European Physical Journal B*, **2016**, 89, 1	1.2	129
224	Superconducting properties of MgB2 from first principles. *Physical Review Letters*, **2005**, 94, 037004	7.4	122
223	Reduced density matrix functional for many-electron systems. *Physical Review B*, **2008**, 78,	3.3	115
222	Laser-induced demagnetization at ultrashort time scales: predictions of TDDFT. *Journal of Chemical Theory and Computation*, **2015**, 11, 4870-4	6.4	114

221	Dynamical Coulomb blockade and the derivative discontinuity of time-dependent density functional theory. *Physical Review Letters*, **2010**, 104, 236801	7.4	109
220	Superconductivity in metastable phases of phosphorus-hydride compounds under high pressure. *Physical Review B*, **2016**, 93,	3.3	108
219	Adiabatic approximation in nonperturbative time-dependent density-functional theory. *Physical Review Letters*, **2008**, 100, 153004	7.4	107
218	Spin-Density Functionals from Current-Density Functional Theory and Vice Versa:A Road towards New Approximations. *Physical Review Letters*, **1997**, 78, 1872-1875	7.4	105
217	Electron correlation energies from scaled exchange-correlation kernels: Importance of spatial versus temporal nonlocality. *Physical Review B*, **2000**, 61, 13431-13437	3.3	105
216	Ab Initio Nonadiabatic Dynamics with Coupled Trajectories: A Rigorous Approach to Quantum (De)Coherence. *Journal of Physical Chemistry Letters*, **2017**, 8, 3048-3055	6.4	101
215	Time-dependent electron localization function. *Physical Review A*, **2005**, 71,	2.6	101
214	Coupled-Trajectory Quantum-Classical Approach to Electronic Decoherence in Nonadiabatic Processes. *Physical Review Letters*, **2015**, 115, 073001	7.4	100
213	Toward the description of van der Waals interactions within density functional theory. *Journal of Computational Chemistry*, **1999**, 20, 12-22	3.5	100
212	Even-harmonic generation due to beyond-Born-Oppenheimer dynamics. *Physical Review Letters*, **2001**, 87, 103901	7.4	96
211	Time-dependent approach to electron pumping in open quantum systems. *Physical Review B*, **2008**, 77,	3.3	94
210	Anisotropic gap of superconducting CaC6: A first-principles density functional calculation. *Physical Review B*, **2007**, 75,	3.3	93
209	Optimal control of quantum rings by terahertz laser pulses. *Physical Review Letters*, **2007**, 98, 157404	7.4	93
208	Strong-field ionization dynamics of a model H2 molecule. *Physical Review A*, **2002**, 65,	2.6	91
207	Quantum-Classical Nonadiabatic Dynamics: Coupled- vs Independent-Trajectory Methods. *Journal of Chemical Theory and Computation*, **2016**, 12, 2127-43	6.4	91
206	Time-Dependent Density Functional Theory beyond Linear Response: An Exchange-Correlation Potential with Memory. *Physical Review Letters*, **1997**, 79, 1905-1908	7.4	90
205	Dynamical steps that bridge piecewise adiabatic shapes in the exact time-dependent potential energy surface. *Physical Review Letters*, **2013**, 110, 263001	7.4	88
204	Spurious interactions, and their correction, in the ensemble-Kohn-Sham scheme for excited States. *Physical Review Letters*, **2002**, 88, 033003	7.4	85

203	Local Density-Functional Theory of Frequency-Dependent Linear Response. *Physical Review Letters*, **1986**, 57, 923-923	7.4	83
202	Is the molecular Berry phase an artifact of the Born-Oppenheimer approximation?. *Physical Review Letters*, **2014**, 113, 263004	7.4	81
201	Density-matrix-power functional: Performance for finite systems and the homogeneous electron gas. *Physical Review A*, **2009**, 79,	2.6	80
200	Thermal conductivity in PbTe from first principles. *Physical Review B*, **2015**, 91,	3.3	77
199	Ab initio angle- and energy-resolved photoelectron spectroscopy with time-dependent density-functional theory. *Physical Review A*, **2012**, 85,	2.6	74
198	Discontinuities of the exchange-correlation kernel and charge-transfer excitations in time-dependent density-functional theory. *Physical Review A*, **2012**, 85,	2.6	74
197	The exact forces on classical nuclei in non-adiabatic charge transfer. *Journal of Chemical Physics*, **2015**, 142, 084303	3.9	73
196	Molecular excitation energies from time-dependent density functional theory. *Computational and Theoretical Chemistry*, **2000**, 501-502, 353-367		69
195	Correlation effects on the third-frequency-moment sum rule of electron liquids. *Physical Review B*, **1987**, 35, 3003-3004	3.3	68
194	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	3	67
193	Correlation potentials for molecular bond dissociation within the self-consistent random phase approximation. *Journal of Chemical Physics*, **2012**, 136, 034106	3.9	67
192	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	7.4	66
191	Exact-exchange density-functional calculations for noble-gas solids. *Physical Review B*, **2004**, 69,	3.3	65
190	Multicomponent density-functional theory for electrons and nuclei. *Physical Review A*, **2008**, 78,	2.6	64
189	Gradient expansion of the Coulomb exchange energy. *Zeitschrift F□ Physik A*, **1981**, 302, 103-106		64
188	Vibrational properties of MnO and NiO from DFT +U-based density functional perturbation theory. *Physical Review B*, **2011**, 84,	3.3	62
187	First-principles approach to noncollinear magnetism: towards spin dynamics. *Physical Review Letters*, **2007**, 98, 196405	7.4	62
186	Optimal control of time-dependent targets. *Physical Review A*, **2005**, 71,	2.6	62

185	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,	3.3	58
184	Two-band superconductivity in Pb from ab initio calculations. *Physical Review B*, **2007**, 75,	3.3	56
183	Time-dependent density-functional theory for superconductors. *Physical Review Letters*, **1994**, 73, 2915-2918	7.4	56
182	Mixed quantum-classical dynamics from the exact decomposition of electron-nuclear motion. *Europhysics Letters*, **2014**, 106, 33001	1.6	55
181	The optimized effective potential method of density functional theory: Applications to atomic and molecular systems. *International Journal of Quantum Chemistry*, **1997**, 64, 95-110	2.1	55
180	Excitation energies from time-dependent density functional theory using exact and approximate potentials. *International Journal of Quantum Chemistry*, **2000**, 80, 534-554	2.1	55
179	Density Functional Theory of Time-Dependent Systems. *NATO ASI Series Series B: Physics*, **1995**, 149-171		55
178	Spectral density and metal-insulator phase transition in Mott insulators within reduced density matrix functional theory. *Physical Review Letters*, **2013**, 110, 116403	7.4	54
177	Thomas-Fermi approach to diatomic systems. I. Solution of the Thomas-Fermi and Thomas-Fermi-Dirac-Weizs□ker equations. *Physical Review A*, **1979**, 20, 1798-1807	2.6	54
176	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	3.9	52
175	Exact conditions in finite-temperature density-functional theory. *Physical Review Letters*, **2011**, 107, 163001	7.4	52
174	Electron-phonon interaction and superconductivity in metallic molecular hydrogen. II. Superconductivity under pressure. *Physical Review B*, **2010**, 81,	3.3	50
173	Classical nuclear motion coupled to electronic non-adiabatic transitions. *Journal of Chemical Physics* , **2014**, 141, 214101	3.9	49
172	Performance of one-body reduced density-matrix functionals for the homogeneous electron gas. *Physical Review B*, **2007**, 75,	3.3	48
171	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	46
170	Molecular geometric phase from the exact electron-nuclear factorization. *Physical Review A*, **2016**, 93,	2.6	43
169	Current density functional theory of spontaneously magnetised solids. *Europhysics Letters*, **1997**, 40, 545-550	1.6	43
168	Tailoring laser pulses with spectral and fluence constraints using optimal control theory. *Journal of Optics B: Quantum and Semiclassical Optics*, **2005**, 7, S300-S312		42

167	Ab initio Eliashberg Theory: Making Genuine Predictions of Superconducting Features. *Journal of the Physical Society of Japan*, **2018**, 87, 041012	1.5	40
166	Ultrafast laser induced local magnetization dynamics in Heusler compounds. *Scientific Reports*, **2016**, 6, 38911	4.9	40
165	Exact Factorization-Based Density Functional Theory of Electrons and Nuclei. *Physical Review Letters*, **2016**, 117, 193001	7.4	39
164	Laser-induced electron localization in H□: mixed quantum-classical dynamics based on the exact time-dependent potential energy surface. *Physical Chemistry Chemical Physics*, **2015**, 17, 29271-80	3.6	39
163	Electron-phonon interaction and superconductivity in metallic molecular hydrogen. I. Electronic and dynamical properties under pressure. *Physical Review B*, **2010**, 81,	3.3	39
162	Scaling and virial theorems in current-density-functional theory. *Physical Review A*, **1996**, 53, R5-R8	2.6	39
161	Accurate solution of the Thomas-Fermi-Dirac-Weizs□ker variational equations for the case of neutral atoms and positive ions. *Zeitschrift F□ Physik A*, **1982**, 309, 5-11		39
160	Electronic Flux Density beyond the Born-Oppenheimer Approximation. *Journal of Physical Chemistry A*, **2016**, 120, 3316-25	2.8	37
159	Electronic Schr□inger equation with nonclassical nuclei. *Physical Review A*, **2014**, 89,	2.6	37
158	Correlation effects in bistability at the nanoscale: Steady state and beyond. *Physical Review B*, **2012**, 85,	3.3	37
157	Superconducting properties of MgB2 from first principles. *Physica C: Superconductivity and Its Applications*, **2007**, 456, 45-53	1.3	37
156	Ab initio prediction of pressure-induced superconductivity in potassium. *Physical Review B*, **2006**, 73,	3.3	37
155	Time-dependent natural orbitals and occupation numbers. *Europhysics Letters*, **2010**, 92, 23001	1.6	36
154	Local Density Approximation for Superconductors. *Physical Review Letters*, **1999**, 83, 2628-2631	7.4	36
153	How Interatomic Steps in the Exact Kohn-Sham Potential Relate to Derivative Discontinuities of the Energy. *Journal of Physical Chemistry Letters*, **2017**, 8, 5974-5980	6.4	35
152	Discontinuity of the chemical potential in reduced-density-matrix-functional theory. *Europhysics Letters*, **2007**, 77, 67003	1.6	35
151	Open shells in reduced-density-matrix-functional theory. *Physical Review A*, **2005**, 72,	2.6	35
150	Response to "Comment on 'Correlated electron-nuclear dynamics: exact factorization of the molecular wavefunction"' [J. Chem. Phys. 139, 087101 (2013)]. *Journal of Chemical Physics*, **2013**, 139, 087102	3.9	34

149	Discontinuities of the Chemical Potential in Reduced Density Matrix Functional Theory. *Zeitschrift Fur Physikalische Chemie*, **2010**, 224, 467-480	3.1	34
148	An exact factorization perspective on quantum interferences in nonadiabatic dynamics. *Journal of Chemical Physics*, **2016**, 145, 034103	3.9	34
147	Orbital magnetism in the density functional theory of superconductors. *Journal De Physique*, **1989**, 50, 2601-2612		33
146	Semiclassical analysis of the electron-nuclear coupling in electronic non-adiabatic processes. *Annalen Der Physik*, **2015**, 527, 546-555	2.6	32
145	Superconducting pairing mediated by spin fluctuations from first principles. *Physical Review B*, **2014** , 90,	3.3	32
144	Transverse spin-gradient functional for noncollinear spin-density-functional theory. *Physical Review Letters*, **2013**, 111, 156401	7.4	32
143	Exchange-energy functionals for finite two-dimensional systems. *Physical Review B*, **2007**, 76,	3.3	32
142	Local measurement of the Eliashberg function of Pb islands: enhancement of electron-phonon coupling by quantum well states. *Physical Review Letters*, **2015**, 114, 047002	7.4	31
141	Femtosecond laser pulse shaping for enhanced ionization. *Europhysics Letters*, **2009**, 87, 53001	1.6	31
140	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	1.3	31
139	Ultrafast demagnetization in bulk versus thin films: an ab initio study. *Journal of Physics Condensed Matter*, **2017**, 29, 224001	1.8	30
138	The optimal one dimensional periodic table: a modified Pettifor chemical scale from data mining. *New Journal of Physics*, **2016**, 18, 093011	2.9	30
137	Exact Single-Electron Approach to the Dynamics of Molecules in Strong Laser Fields. *Physical Review Letters*, **2017**, 118, 163202	7.4	30
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	3.9	30
135	Electronic structure via potential functional approximations. *Physical Review Letters*, **2011**, 106, 236404	7.4	30
134	Optimal laser control of double quantum dots. *Physical Review B*, **2008**, 77,	3.3	30
133	An efficient algorithm for time propagation as applied to linearized augmented plane wave method. *Computer Physics Communications*, **2016**, 209, 92-95	4.2	30
132	Large magnetocrystalline anisotropy in tetragonally distorted Heuslers: a systematic study. *Journal Physics D: Applied Physics*, **2017**, 50, 095002	3	29

131	The role of Coulomb interaction in the superconducting properties of CaC6and H under pressure. *Superconductor Science and Technology*, **2009**, 22, 034006	3.1	29
130	Resonant inelastic soft x-ray scattering of Be chalcogenides. *Physical Review B*, **2006**, 73,	3.3	29
129	Asymptotic Properties of the Optimized Effective Potential. *Advances in Quantum Chemistry*, **1998**, 31-48	1.4	29
128	Optimization schemes for selective molecular cleavage with tailored ultrashort laser pulses. *Chemical Physics*, **2011**, 391, 50-61	2.3	28
127	Bound states in time-dependent quantum transport: oscillations and memory effects in current and density. *Physical Chemistry Chemical Physics*, **2009**, 11, 4535-8	3.6	28
126	Time-dependent electron localization functions for coupled nuclear-electronic motion. *Journal of Chemical Physics*, **2004**, 121, 9666-70	3.9	28
125	Relativistic framework for microscopic theories of superconductivity. I. The Dirac equation for superconductors. *Physical Review B*, **1999**, 59, 7140-7154	3.3	28
124	Spin-multiplet energies from time-dependent density functional theory. *International Journal of Quantum Chemistry*, **1996**, 60, 1393-1401	2.1	28
123	Ensemble-Density functional theory for excited states. *International Journal of Quantum Chemistry*, **1990**, 38, 707-716	2.1	28
122	Time-dependent density-functional and reduced density-matrix methods for few electrons: Exact versus adiabatic approximations. *Chemical Physics*, **2011**, 391, 1-10	2.3	27
121	Multicomponent density-functional theory for time-dependent systems. *Physical Review A*, **2007**, 76,	2.6	27
120	Paramagnons in FeSe close to a magnetic quantum phase transition: Ab initio study. *Physical Review B*, **2012**, 86,	3.3	26
119	Discrete peaks in above-threshold double-ionization spectra. *Physical Review A*, **2001**, 64,	2.6	26
118	Competing Spin Transfer and Dissipation at Co/Cu(001) Interfaces on Femtosecond Timescales. *Physical Review Letters*, **2019**, 122, 067202	7.4	25
117	Electronic, vibrational, and superconducting properties of CaBeSi: First-principles calculations. *Physical Review B*, **2009**, 79,	3.3	25
116	Correlation energy of finite two-dimensional systems: Toward nonempirical and universal modeling. *Physical Review B*, **2009**, 79,	3.3	25
115	Comparison of exact-exchange calculations for solids in current-spin-density- and spin-density-functional theory. *Physical Review B*, **2007**, 76,	3.3	25
114	Reversible Formation of 2D Electron Gas at the LaFeO /SrTiO Interface via Control of Oxygen Vacancies. *Advanced Materials*, **2017**, 29, 1604447	24	24

113	Ab initio theory of iron-based superconductors. *Physical Review B*, **2016**, 94,	3.3	24
112	Phononic self-energy effects and superconductivity in CaC6. *Physical Review B*, **2012**, 85,	3.3	24
111	The role of bound states in time-dependent quantum transport. *Applied Physics A: Materials Science and Processing*, **2008**, 93, 355-364	2.6	24
110	Time-dependent variational approach to molecules in strong laser fields. *Chemical Physics*, **2004**, 304, 183-202	2.3	24
109	Optimal control of laser-induced spin–orbit mediated ultrafast demagnetization. *New Journal of Physics*, **2016**, 18, 013014	2.9	24
108	Enhancing and controlling single-atom high-harmonic generation spectra: a time-dependent density-functional scheme. *European Physical Journal B*, **2015**, 88, 1	1.2	23
107	First-Principles Calculation of the Real-Space Order Parameter and Condensation Energy Density in Phonon-Mediated Superconductors. *Physical Review Letters*, **2015**, 115, 097002	7.4	23
106	Magnon spectrum of transition-metal oxides: Calculations including long-range magnetic interactions using the LSDA+U method. *Physical Review B*, **2011**, 84,	3.3	23
105	Gaussian approximations for the exchange-energy functional of current-carrying states: Applications to two-dimensional systems. *Physical Review A*, **2009**, 80,	2.6	23
104	Optimized effective potential method in current-spin-density-functional theory. *Physical Review A*, **2006**, 74,	2.6	23
103	Thomas-Fermi approach to diatomic systems. II. Correlation diagrams for N-N and Ne-Ne. *Physical Review A*, **1979**, 20, 1808-1815	2.6	23
102	A guided tour of time-dependent density functional theory **1998**, 116-146		22
101	Exchange-correlation orbital functionals in current-density functional theory: Application to a quantum dot in magnetic fields. *Physical Review B*, **2008**, 77,	3.3	22
100	On the Mass of Atoms in Molecules: Beyond the Born-Oppenheimer Approximation. *Physical Review X*, **2017**, 7,	9.1	21
99	Discontinuous functional for linear-response time-dependent density-functional theory: The exact-exchange kernel and approximate forms. *Physical Review A*, **2013**, 88,	2.6	21
98	Ensemble-Hartree–Fock scheme for excited states. The optimized effective potential method. *Physica B: Condensed Matter*, **2002**, 318, 328-332	2.8	21
97	Optimal control of strong-field ionization with time-dependent density-functional theory. *Physical Review A*, **2013**, 88,	2.6	20
96	Discontinuity of the chemical potential in reduced-density-matrix-functional theory for open-shell systems. *Physical Review A*, **2009**, 79,	2.6	20

95	Electronic exchange in quantum rings: Beyond the local-density approximation. *Physical Review B*, **2009**, 79,	3.3	20
94	Chapter 10 Time-dependent transport phenomena. *Theoretical and Computational Chemistry*, **2007**, 17, 247-284		20
93	Density-functional theory of the superconducting state. *International Journal of Quantum Chemistry* , **1991**, 40, 289-297	2.1	19
92	Optical response of extended systems using time-dependent density functional theory. *Topics in Current Chemistry*, **2014**, 347, 235-57		18
91	Multiplicity of solutions to GW-type approximations. *Physical Review B*, **2015**, 92,	3.3	18
90	Theoretical investigation of optical conductivity in Ba(Fe1−xCox)2As2. *Physical Review B*, **2011**, 83,	3.3	18
89	Theory of Dichroism in the Electromagnetic Response of Superconductors. *Physical Review Letters*, **1997**, 78, 3753-3756	7.4	18
88	Approximate relativistic optimized potential method. *Physical Review A*, **1998**, 57, 138-148	2.6	18
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86	Electron-nuclear wave-packet dynamics through a conical intersection. *Journal of Chemical Physics*, **2017**, 146, 074304	3.9	17
85	Density functional theory of electron transfer beyond the Born-Oppenheimer approximation: Case study of LiF. *Journal of Chemical Physics*, **2018**, 148, 084110	3.9	17
84	Potential functionals versus density functionals. *Physical Review A*, **2013**, 88,	2.6	17
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82	Reduced-density-matrix-functional theory at finite temperature: Theoretical foundations. *Physical Review A*, **2015**, 92,	2.6	17
81	Conventional Quantum Chemical Correlation Energy Versus Density-Functional Correlation Energy. *ACS Symposium Series*, **1996**, 42-53	0.4	17
80	Ab initio theory of superconductivity in a magnetic field. I. Spin density functional theory for superconductors and Eliashberg equations. *Physical Review B*, **2015**, 92,	3.3	16
79	Asymptotic analysis of the Berry curvature in the E?e Jahn-Teller model. *Physical Review A*, **2017**, 96,	2.6	16
78	Spectrum for nonmagnetic mott insulators from power functional within reduced density matrix functional theory. *Journal of Chemical Theory and Computation*, **2015**, 11, 4895-9	6.4	16

77	Adiabatic Connection and the Kohn-Sham Variety of Potential-Functional Theory. *Journal of Chemical Theory and Computation*, **2009**, 5, 844-9	6.4	16
76	Phase-space analysis of double ionization. *Optics Express*, **2001**, 8, 411-6	3.3	16
75	Ab initio theory of superconductivity in a magnetic field. II. Numerical solution. *Physical Review B*, **2015**, 92,	3.3	15
74	Source-Free Exchange-Correlation Magnetic Fields in Density Functional Theory. *Journal of Chemical Theory and Computation*, **2018**, 14, 1247-1253	6.4	15
73	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	15
72	Measuring the kernel of time-dependent density functional theory with x-ray absorption spectroscopy of transition metals. *Physical Review Letters*, **2005**, 95, 253006	7.4	15
71	First-principles study of rare-earth-doped superconducting CaFe2As2. *Physical Review B*, **2012**, 86,	3.3	14
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69	Electron localization function for two-dimensional systems. *Physical Review B*, **2008**, 77,	3.3	14
68	Density functional theory for superconductors. *International Journal of Quantum Chemistry*, **2004**, 99, 790-797	2.1	14
67	Relativistic framework for microscopic theories of superconductivity. II. The Pauli equation for superconductors. *Physical Review B*, **1999**, 59, 7155-7165	3.3	14
66	Thomas-Fermi potentials for quasimolecular collision processes. *Physics Letters, Section A: General, Atomic and Solid State Physics*, **1976**, 57, 131-134	2.3	14
65	Effect of discontinuities in Kohn-Sham-based chemical reactivity theory. *Journal of Chemical Physics* , **2012**, 136, 114102	3.9	12
64	Analysis of dichroism in the electromagnetic response of superconductors. *Physical Review B*, **1998**, 58, 473-489	3.3	12
63	Functionals of fractional form in variational scattering theory. *Physical Review A*, **1982**, 26, 3004-3007	2.6	12
62	Excitons in Organics Using Time-Dependent Density Functional Theory: PPV, Pentacene, and Picene. *Journal of Chemical Theory and Computation*, **2015**, 11, 1710-4	6.4	11
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