Eberhard K U Gross

List of Publications by Year in Descending Order

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	Energy, Momentum, and Angular Momentum Transfer between Electrons and Nuclei.. *Physical Review Letters*, **2022**, 128, 113001	7.4	1
255	Geometric energy transfer in two-component systems.. *Philosophical Transactions Series A, Mathematical, Physical, and Engineering Sciences*, **2022**, 380, 20200383	3	2
254	Fock-Space Embedding Theory: Application to Strongly Correlated Topological Phases. *Physical Review Letters*, **2021**, 127, 116401	7.4	2
253	The 2021 Room-Temperature Superconductivity Roadmap. *Journal of Physics Condensed Matter*, **2021**,	1.8	9
252	Many-body Green's function theory of electrons and nuclei beyond the Born-Oppenheimer approximation. *Physical Review B*, **2020**, 101,	3.3	3
251	Generation of magnetic skyrmions by focused vortex laser pulses. *Journal of Applied Physics*, **2020**, 127, 073904	2.5	10
250	Electron-nuclear entanglement in the time-dependent molecular wavefunction. *Computational and Theoretical Chemistry*, **2019**, 1151, 99-106	2	10
249	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	1
248	Exact factorization-based density functional theory of electron-phonon systems. *Physical Review B*, **2019**, 99,	3.3	10
247	Model Hamiltonian for strongly correlated systems: Systematic, self-consistent, and unique construction. *Physical Review B*, **2019**, 99,	3.3	7
246	Competing Spin Transfer and Dissipation at Co/Cu(001) Interfaces on Femtosecond Timescales. *Physical Review Letters*, **2019**, 122, 067202	7.4	25
245	Complete description of the magnetic ground state in spinel vanadates. *Physical Review B*, **2019**, 100,	3.3	1
244	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
243	IR and NMR spectroscopic correlation of enterobactin by DFT. *Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy*, **2018**, 198, 264-277	4.4	8
242	Ab initio Eliashberg Theory: Making Genuine Predictions of Superconducting Features. *Journal of the Physical Society of Japan*, **2018**, 87, 041012	1.5	40
241	Source-Free Exchange-Correlation Magnetic Fields in Density Functional Theory. *Journal of Chemical Theory and Computation*, **2018**, 14, 1247-1253	6.4	15
240	Controlling observables in normal, hybrid and Josephson junctions. *Molecular Physics*, **2018**, 116, 2449-2460		

239	Accurate Formula for the Macroscopic Polarization of Strongly Correlated Materials. *Journal of Physical Chemistry Letters*, **2018**, 9, 7045-7051	6.4	5
238	Experimental and theoretical structural/spectroscopical correlation of enterobactin and catecholamide. *Data in Brief*, **2018**, 20, 2054-2064	1.2	1
237	Ab initio study of doping effects in the 42214 compounds: A new family of layered iron-based superconductors. *Physical Review B*, **2017**, 95,	3.3	1
236	Reversible Formation of 2D Electron Gas at the LaFeO /SrTiO Interface via Control of Oxygen Vacancies. *Advanced Materials*, **2017**, 29, 1604447	24	24
235	Electron-nuclear wave-packet dynamics through a conical intersection. *Journal of Chemical Physics*, **2017**, 146, 074304	3.9	17
234	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
233	Ultrafast demagnetization in bulk versus thin films: an ab initio study. *Journal of Physics Condensed Matter*, **2017**, 29, 224001	1.8	30
232	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
231	On the Mass of Atoms in Molecules: Beyond the Born-Oppenheimer Approximation. *Physical Review X*, **2017**, 7,	9.1	21
230	L10 Stacked Binaries as Candidates for Hard-Magnets: FePt, MnAl and MnGa. *Annalen Der Physik*, **2017**, 529, 1600412	2.6	3
229	Large magnetocrystalline anisotropy in tetragonally distorted Heuslers: a systematic study. *Journal Physics D: Applied Physics*, **2017**, 50, 095002	3	29
228	Exact Single-Electron Approach to the Dynamics of Molecules in Strong Laser Fields. *Physical Review Letters*, **2017**, 118, 163202	7.4	30
227	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
226	Spin-density fluctuations and the fluctuation-dissipation theorem in 3d ferromagnetic metals. *Physical Review B*, **2017**, 96,	3.3	7
225	Surface hopping in laser-driven molecular dynamics. *Physical Review A*, **2017**, 95,	2.6	17
224	Asymptotic analysis of the Berry curvature in the E?e Jahn-Teller model. *Physical Review A*, **2017**, 96,	2.6	16
223	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,	2.6	4
222	Molecular geometric phase from the exact electron-nuclear factorization. *Physical Review A*, **2016**, 93,	2.6	43

221	Superconductivity in metastable phases of phosphorus-hydride compounds under high pressure. *Physical Review B*, **2016**, 93,	3.3	108
220	42214 layered Fe-based superconductors: An ab initio study of their structural, magnetic, and electronic properties. *Physical Review B*, **2016**, 93,	3.3	3
219	Ab initio theory of iron-based superconductors. *Physical Review B*, **2016**, 94,	3.3	24
218	Exact Factorization-Based Density Functional Theory of Electrons and Nuclei. *Physical Review Letters*, **2016**, 117, 193001	7.4	39
217	The optimal one dimensional periodic table: a modified Pettifor chemical scale from data mining. *New Journal of Physics*, **2016**, 18, 093011	2.9	30
216	Swift thermal steering of domain walls in ferromagnetic MnBi stripes. *Scientific Reports*, **2016**, 6, 24411	4.9	9
215	Ultrafast laser induced local magnetization dynamics in Heusler compounds. *Scientific Reports*, **2016**, 6, 38911	4.9	40
214	High temperature superconductivity in sulfur and selenium hydrides at high pressure. *European Physical Journal B*, **2016**, 89, 1	1.2	129
213	Reproducibility in density functional theory calculations of solids. *Science*, **2016**, 351, aad3000	33.3	784
212	Electronic Flux Density beyond the Born-Oppenheimer Approximation. *Journal of Physical Chemistry A*, **2016**, 120, 3316-25	2.8	37
211	Optimal control of laser-induced spin□rbit mediated ultrafast demagnetization. *New Journal of Physics*, **2016**, 18, 013014	2.9	24
210	An exact factorization perspective on quantum interferences in nonadiabatic dynamics. *Journal of Chemical Physics*, **2016**, 145, 034103	3.9	34
209	Quantum-Classical Nonadiabatic Dynamics: Coupled- vs Independent-Trajectory Methods. *Journal of Chemical Theory and Computation*, **2016**, 12, 2127-43	6.4	91
208	An efficient algorithm for time propagation as applied to linearized augmented plane wave method. *Computer Physics Communications*, **2016**, 209, 92-95	4.2	30
207	Comment on "Estimating Excitonic Effects in the Absorption Spectra of Solids: Problems and Insight from a Guided Iteration Scheme". *Physical Review Letters*, **2016**, 117, 159701	7.4	4
206	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
205	The exact forces on classical nuclei in non-adiabatic charge transfer. *Journal of Chemical Physics*, **2015**, 142, 084303	3.9	73
204	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

203	Ab initio theory of superconductivity in a magnetic field. II. Numerical solution. *Physical Review B*, **2015**, 92,	3.3	15
202	Thermal conductivity in PbTe from first principles. *Physical Review B*, **2015**, 91,	3.3	77
201	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
200	Laser-induced demagnetization at ultrashort time scales: predictions of TDDFT. *Journal of Chemical Theory and Computation*, **2015**, 11, 4870-4	6.4	114
199	Almost exact exchange at almost no computational cost in electronic structure. *Physical Review A*, **2015**, 92,	2.6	6
198	Reduced-density-matrix-functional theory at finite temperature: Theoretical foundations. *Physical Review A*, **2015**, 92,	2.6	17
197	Multiplicity of solutions to GW-type approximations. *Physical Review B*, **2015**, 92,	3.3	18
196	Coupled-Trajectory Quantum-Classical Approach to Electronic Decoherence in Nonadiabatic Processes. *Physical Review Letters*, **2015**, 115, 073001	7.4	100
195	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
194	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
193	Doping induced metal-insulator phase transition in NiO□ reduced density matrix functional theory perspective. *New Journal of Physics*, **2015**, 17, 093038	2.9	10
192	Semiclassical analysis of the electron-nuclear coupling in electronic non-adiabatic processes. *Annalen Der Physik*, **2015**, 527, 546-555	2.6	32
191	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
190	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
189	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
188	Electronic Schr□dinger equation with nonclassical nuclei. *Physical Review A*, **2014**, 89,	2.6	37
187	How to represent crystal structures for machine learning: Towards fast prediction of electronic properties. *Physical Review B*, **2014**, 89,	3.3	275
186	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

185	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	11
184	Optical response of extended systems using time-dependent density functional theory. *Topics in Current Chemistry*, **2014**, 347, 235-57		18
183	Mixed quantum-classical dynamics from the exact decomposition of electron-nuclear motion. *Europhysics Letters*, **2014**, 106, 33001	1.6	55
182	Virial theorem and exact properties of density functionals for periodic systems. *Physical Review B*, **2014**, 89,	3.3	1
181	Is the molecular Berry phase an artifact of the Born-Oppenheimer approximation?. *Physical Review Letters*, **2014**, 113, 263004	7.4	81
180	Classical nuclear motion coupled to electronic non-adiabatic transitions. *Journal of Chemical Physics* , **2014**, 141, 214101	3.9	49
179	Superconducting pairing mediated by spin fluctuations from first principles. *Physical Review B*, **2014** , 90,	3.3	32
178	Potential functionals versus density functionals. *Physical Review A*, **2013**, 88,	2.6	17
177	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
176	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
175	Minimization procedure in reduced density matrix functional theory by means of an effective noninteracting system. *Computational and Theoretical Chemistry*, **2013**, 1003, 114-122	2	8
174	Dynamical steps that bridge piecewise adiabatic shapes in the exact time-dependent potential energy surface. *Physical Review Letters*, **2013**, 110, 263001	7.4	88
173	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
172	Transverse spin-gradient functional for noncollinear spin-density-functional theory. *Physical Review Letters*, **2013**, 111, 156401	7.4	32
171	Optimal control of strong-field ionization with time-dependent density-functional theory. *Physical Review A*, **2013**, 88,	2.6	20
170	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
169	First-principles study of rare-earth-doped superconducting CaFe2As2. *Physical Review B*, **2012**, 86,	3.3	14
168	Ab initio angle- and energy-resolved photoelectron spectroscopy with time-dependent density-functional theory. *Physical Review A*, **2012**, 85,	2.6	74

167	Paramagnons in FeSe close to a magnetic quantum phase transition: Ab initio study. *Physical Review B*, **2012**, 86,	3.3	26
166	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
165	Correlated electron-nuclear dynamics: exact factorization of the molecular wavefunction. *Journal of Chemical Physics*, **2012**, 137, 22A530	3.9	157
164	Ionization potentials and electron affinities from reduced-density-matrix functional theory. *Physical Review A*, **2012**, 85,	2.6	14
163	Fundamentals of Time-Dependent Density Functional Theory. *Lecture Notes in Physics*, **2012**,	0.8	277
162	Effect of discontinuities in Kohn-Sham-based chemical reactivity theory. *Journal of Chemical Physics* , **2012**, 136, 114102	3.9	12
161	Correlation potentials for molecular bond dissociation within the self-consistent random phase approximation. *Journal of Chemical Physics*, **2012**, 136, 034106	3.9	67
160	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
159	Discontinuities of the exchange-correlation kernel and charge-transfer excitations in time-dependent density-functional theory. *Physical Review A*, **2012**, 85,	2.6	74
158	Correlation effects in bistability at the nanoscale: Steady state and beyond. *Physical Review B*, **2012**, 85,	3.3	37
157	Phononic self-energy effects and superconductivity in CaC6. *Physical Review B*, **2012**, 85,	3.3	24
156	Bootstrap approximation for the exchange-correlation kernel of time-dependent density-functional theory. *Physical Review Letters*, **2011**, 107, 186401	7.4	131
155	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
154	Exact conditions in finite-temperature density-functional theory. *Physical Review Letters*, **2011**, 107, 163001	7.4	52
153	Vibrational properties of MnO and NiO from DFT +U-based density functional perturbation theory. *Physical Review B*, **2011**, 84,	3.3	62
152	Optimization schemes for selective molecular cleavage with tailored ultrashort laser pulses. *Chemical Physics*, **2011**, 391, 50-61	2.3	28
151	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
150	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

149	Electronic structure via potential functional approximations. *Physical Review Letters*, **2011**, 106, 236404	7.4	30
148	Theoretical investigation of optical conductivity in Ba(Fe1−xCox)2As2. *Physical Review B*, **2011**, 83,	3.3	18
147	Electron-phonon interaction and superconductivity in metallic molecular hydrogen. I. Electronic and dynamical properties under pressure. *Physical Review B*, **2010**, 81,	3.3	39
146	Noncollinear spin-spiral phase for the uniform electron gas within reduced-density-matrix-functional theory. *Physical Review B*, **2010**, 81,	3.3	7
145	Static and dynamical susceptibility of LaO1−xFxFeAs. *Physical Review B*, **2010**, 81,	3.3	6
144	Time-dependent natural orbitals and occupation numbers. *Europhysics Letters*, **2010**, 92, 23001	1.6	36
143	Dynamical Coulomb blockade and the derivative discontinuity of time-dependent density functional theory. *Physical Review Letters*, **2010**, 104, 236801	7.4	109
142	Exact factorization of the time-dependent electron-nuclear wave function. *Physical Review Letters*, **2010**, 105, 123002	7.4	285
141	Electron-phonon interaction and superconductivity in metallic molecular hydrogen. II. Superconductivity under pressure. *Physical Review B*, **2010**, 81,	3.3	50
140	Discontinuities of the Chemical Potential in Reduced Density Matrix Functional Theory. *Zeitschrift Fur Physikalische Chemie*, **2010**, 224, 467-480	3.1	34
139	Transport properties of chrysazine-type molecules. *Theoretical Chemistry Accounts*, **2010**, 125, 535-541	1.9	1
138	Acceleration of quantum optimal control theory algorithms with mixing strategies. *Physical Review E*, **2009**, 79, 056704	2.4	8
137	Magnetism in CeFeAsO1−xFx and LaFeAsO1−xFx from first principles. *Physical Review B*, **2009**, 80,	3.3	11
136	Discontinuity of the chemical potential in reduced-density-matrix-functional theory for open-shell systems. *Physical Review A*, **2009**, 79,	2.6	20
135	Electronic exchange in quantum rings: Beyond the local-density approximation. *Physical Review B*, **2009**, 79,	3.3	20
134	Gaussian approximations for the exchange-energy functional of current-carrying states: Applications to two-dimensional systems. *Physical Review A*, **2009**, 80,	2.6	23
133	Electronic, vibrational, and superconducting properties of CaBeSi: First-principles calculations. *Physical Review B*, **2009**, 79,	3.3	25
132	Correlation energy of finite two-dimensional systems: Toward nonempirical and universal modeling. *Physical Review B*, **2009**, 79,	3.3	25

131	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
130	Multiband superconductivity in Pb, H under pressure and CaBeSi from ab initio calculations. *Journal of Physics Condensed Matter*, **2009**, 21, 164209	1.8	9
129	Density functional theory for superconductors. *International Journal of Quantum Chemistry*, **2009**, 36, 611-615	2.1	
128	Adiabatic Connection and the Kohn-Sham Variety of Potential-Functional Theory. *Journal of Chemical Theory and Computation*, **2009**, 5, 844-9	6.4	16
127	Femtosecond laser pulse shaping for enhanced ionization. *Europhysics Letters*, **2009**, 87, 53001	1.6	31
126	The role of Coulomb interaction in the superconducting properties of CaC6and H under pressure. *Superconductor Science and Technology*, **2009**, 22, 034006	3.1	29
125	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
124	Density-matrix-power functional: Performance for finite systems and the homogeneous electron gas. *Physical Review A*, **2009**, 79,	2.6	80
123	Adiabatic approximation in nonperturbative time-dependent density-functional theory. *Physical Review Letters*, **2008**, 100, 153004	7.4	107
122	Reduced density matrix functional for many-electron systems. *Physical Review B*, **2008**, 78,	3.3	115
121	Electron localization function for two-dimensional systems. *Physical Review B*, **2008**, 77,	3.3	14
120	Time-dependent approach to electron pumping in open quantum systems. *Physical Review B*, **2008**, 77,	3.3	94
119	Optimal laser control of double quantum dots. *Physical Review B*, **2008**, 77,	3.3	30
118	Ab initio description of high-temperature superconductivity in dense molecular hydrogen. *Physical Review Letters*, **2008**, 100, 257001	7.4	167
117	Publisher Note: Ab initio Description of High-Temperature Superconductivity in Dense Molecular Hydrogen [Phys. Rev. Lett. 100, 257001 (2008)]. *Physical Review Letters*, **2008**, 101,	7.4	3
116	Multicomponent density-functional theory for electrons and nuclei. *Physical Review A*, **2008**, 78,	2.6	64
115	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
114	The role of bound states in time-dependent quantum transport. *Applied Physics A: Materials Science and Processing*, **2008**, 93, 355-364	2.6	24

113	Coherent quantum switch driven by optimized laser pulses. *Physica E: Low-Dimensional Systems and Nanostructures*, **2008**, 40, 1593-1595	3	4
112	Anisotropic gap of superconducting CaC6: A first-principles density functional calculation. *Physical Review B*, **2007**, 75,	3.3	93
111	XMCD Analysis Beyond Standard Procedures. *AIP Conference Proceedings*, **2007**,	0	10
110	Superconducting properties of MgB2 from first principles. *Physica C: Superconductivity and Its Applications*, **2007**, 456, 45-53	1.3	37
109	Orbital currents in the Colle-Salvetti correlation energy functional and the degeneracy problem. *Journal of Chemical Physics*, **2007**, 127, 124103	3.9	9
108	Two-band superconductivity in Pb from ab initio calculations. *Physical Review B*, **2007**, 75,	3.3	56
107	Multicomponent density-functional theory for time-dependent systems. *Physical Review A*, **2007**, 76,	2.6	27
106	Comparison of exact-exchange calculations for solids in current-spin-density- and spin-density-functional theory. *Physical Review B*, **2007**, 76,	3.3	25
105	First-principles approach to noncollinear magnetism: towards spin dynamics. *Physical Review Letters*, **2007**, 98, 196405	7.4	62
104	Performance of one-body reduced density-matrix functionals for the homogeneous electron gas. *Physical Review B*, **2007**, 75,	3.3	48
103	Exchange-energy functionals for finite two-dimensional systems. *Physical Review B*, **2007**, 76,	3.3	32
102	Optimal control of quantum rings by terahertz laser pulses. *Physical Review Letters*, **2007**, 98, 157404	7.4	93
101	Chapter 10 Time-dependent transport phenomena. *Theoretical and Computational Chemistry*, **2007**, 17, 247-284		20
100	Discontinuity of the chemical potential in reduced-density-matrix-functional theory. *Europhysics Letters*, **2007**, 77, 67003	1.6	35
99	Quantum optimal control theory. *Journal of Physics B: Atomic, Molecular and Optical Physics*, **2007**, 40, R175-R211	1.3	258
98	Molecules and clusters in strong laser fields **2007**, 485-617		2
97	On the degeneracy of atomic states within exact-exchange (spin-) density functional theory. *Journal of Chemical Physics*, **2006**, 125, 084105	3.9	11
96	Back to the Ground-State: Electron Gas. *Lecture Notes in Physics*, **2006**, 423-434	0.8	2

95	Multicomponent Density-Functional Theory. *Lecture Notes in Physics*, **2006**, 93-106	0.8	6
94	Optimized effective potential method in current-spin-density-functional theory. *Physical Review A*, **2006**, 74,	2.6	23
93	Superconductivity in lithium, potassium, and aluminum under extreme pressure: a first-principles study. *Physical Review Letters*, **2006**, 96, 047003	7.4	138
92	Resonant inelastic soft x-ray scattering of Be chalcogenides. *Physical Review B*, **2006**, 73,	3.3	29
91	Ab initio prediction of pressure-induced superconductivity in potassium. *Physical Review B*, **2006**, 73,	3.3	37
90	Exact Coulomb cutoff technique for supercell calculations. *Physical Review B*, **2006**, 73,	3.3	286
89	Optimal control of charge transfer **2006**, 6325, 114		1
88	Double-pole approximation in time-dependent density functional theory. *International Journal of Quantum Chemistry*, **2006**, 106, 2840-2847	2.1	6
87	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
86	Ab initio theory of superconductivity. II. Application to elemental metals. *Physical Review B*, **2005**, 72,	3.3	199
85	Ab initio theory of superconductivity. I. Density functional formalism and approximate functionals. *Physical Review B*, **2005**, 72,	3.3	237
84	Time-dependent density functional theory: past, present, and future. *Journal of Chemical Physics*, **2005**, 123, 62206	3.9	665
83	Time-dependent quantum transport: A practical scheme using density functional theory. *Physical Review B*, **2005**, 72,	3.3	275
82	Ab-initio Computation of Superconducting Properties of Elemental Superconductors and MgB2. *Journal of Superconductivity and Novel Magnetism*, **2005**, 18, 649-652		1
81	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
80	Time-dependent electron localization function. *Physical Review A*, **2005**, 71,	2.6	101
79	Superconducting properties of MgB2 from first principles. *Physical Review Letters*, **2005**, 94, 037004	7.4	122
78	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

77	Open shells in reduced-density-matrix-functional theory. *Physical Review A*, **2005**, 72,	2.6	35
76	Optimal control of time-dependent targets. *Physical Review A*, **2005**, 71,	2.6	62
75	Time-dependent density functional theory. *Annual Review of Physical Chemistry*, **2004**, 55, 427-55	15.7	932
74	Density functional theory for superconductors. *International Journal of Quantum Chemistry*, **2004**, 99, 790-797	2.1	14
73	Time-dependent variational approach to molecules in strong laser fields. *Chemical Physics*, **2004**, 304, 183-202	2.3	24
72	Time-dependent electron localization functions for coupled nuclear-electronic motion. *Journal of Chemical Physics*, **2004**, 121, 9666-70	3.9	28
71	Exact-exchange density-functional calculations for noble-gas solids. *Physical Review B*, **2004**, 69,	3.3	65
70	Excitations in time-dependent density-functional theory. *Physical Review Letters*, **2003**, 90, 043005	7.4	148
69	Towards Time-Dependent Density-Functional Theory for Molecules in Strong Laser Pulses. *Progress in Theoretical Chemistry and Physics*, **2003**, 69-77	0.6	4
68	Ensemble-HartreeFock scheme for excited states. The optimized effective potential method. *Physica B: Condensed Matter*, **2002**, 318, 328-332	2.8	21
67	Strong-field ionization dynamics of a model H2 molecule. *Physical Review A*, **2002**, 65,	2.6	91
66	Spurious interactions, and their correction, in the ensemble-Kohn-Sham scheme for excited States. *Physical Review Letters*, **2002**, 88, 033003	7.4	85
65	Discrete peaks in above-threshold double-ionization spectra. *Physical Review A*, **2001**, 64,	2.6	26
64	Even-harmonic generation due to beyond-Born-Oppenheimer dynamics. *Physical Review Letters*, **2001**, 87, 103901	7.4	96
63	Phase-space analysis of double ionization. *Optics Express*, **2001**, 8, 411-6	3.3	16
62	Multicomponent density-functional theory for electrons and nuclei. *Physical Review Letters*, **2001**, 86, 2984-7	7.4	183
61	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
60	Molecular excitation energies from time-dependent density functional theory. *Computational and Theoretical Chemistry*, **2000**, 501-502, 353-367		69

59	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
58	Electron correlation energies from scaled exchange-correlation kernels: Importance of spatial versus temporal nonlocality. *Physical Review B*, **2000**, 61, 13431-13437	3.3	105
57	Intense-field double ionization of helium: identifying the mechanism. *Physical Review Letters*, **2000**, 85, 4707-10	7.4	255
56	Local Density Approximation for Superconductors. *Physical Review Letters*, **1999**, 83, 2628-2631	7.4	36
55	Theory of relativistic effects in superconductors. *Physica C: Superconductivity and Its Applications*, **1999**, 317-318, 508-510	1.3	1
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