Angel Rubio

List of Publications by Year
in descending order

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407 papers	37,234 citations	2675 95 h-index	3650 180 g-index
413 all docs	413 docs citations	413 times ranked	24808 citing authors

#	Article	IF	Citations
1	Free electron gas in cavity quantum electrodynamics. Physical Review Research, 2022, 4, .	3.6	33
2	Detecting multiple chiral centers in chiral molecules with high harmonic generation. Optics Express, 2022, 30, 3729.	3.4	16
3	MoirÃ© engineering of spinâ€“orbit coupling in twisted platinum diselenide. Electronic Structure, 2022, 4, 014004.	2.8	8
4	First-principles modelling for time-resolved ARPES under different pumpâ€“probe conditions. Journal of Electron Spectroscopy and Related Phenomena, 2022, 254, 147152.	1.7	9
5	Nanometer-Scale Lateral pâ€“n Junctions in Graphene/Î±-RuCl₃ Heterostructures. Nano Letters, 2022, 22, 1946-1953.	9.1	25
6	Cavity-Modulated Proton Transfer Reactions. Journal of the American Chemical Society, 2022, 144, 4995-5002.	13.7	32
7	TMDs as a platform for spin liquid physics: A strong coupling study of twisted bilayer WSe2. APL Materials, 2022, 10, .	5.1	19
8	A new Hall for quantum protection. Science, 2022, 375, 976-977.	12.6	4
9	Microscopic theory of light-induced ultrafast skyrmion excitation in transition metal films. Npj Computational Materials, 2022, 8, .	8.7	8
10	Comment on â€œOrigin of symmetry-forbidden high-order harmonic generation in the time-dependent Kohn-Sham formulationâ€• Physical Review A, 2022, 105, .	2.5	1
11	MoirÃ© nematic phase in twisted double bilayer graphene. Nature Physics, 2022, 18, 196-202.	16.7	51
12	Polaritonic Hofstadter butterfly and cavity control of the quantized Hall conductance. Physical Review B, 2022, 105, .	3.2	20
13	A perspective on ab initio modeling of polaritonic chemistry: The role of non-equilibrium effects and quantum collectivity. Journal of Chemical Physics, 2022, 156, .	3.0	39
14	Strongly correlated electronâ€“photon systems. Nature, 2022, 606, 41-48.	27.8	66
15	Probing phonon dynamics with multidimensional high harmonic carrier-envelope-phase spectroscopy. Proceedings of the National Academy of Sciences of the United States of America, 2022, 119, .	7.1	13
16	Frequency-Dependent Sternheimer Linear-Response Formalism for Strongly Coupled Lightâ€“Matter Systems. Journal of Chemical Theory and Computation, 2022, 18, 4354-4365.	5.3	9
17	Effect of spin-orbit coupling on the high harmonics from the topological Dirac semimetal Na3Bi. Npj Computational Materials, 2022, 8, .	8.7	13
18	Engineering quantum materials with chiral optical cavities. Nature Materials, 2021, 20, 438-442.	27.5	120

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19	Toward Confined Carbyne with Tailored Properties. Nano Letters, 2021, 21, 1096-1101.	9.1	27
20	MoirÃ© metrology of energy landscapes in van der Waals heterostructures. Nature Communications, 2021, 12, 242.	12.8	60
21	Vibrational coherent control of localized dâ€“d electronic excitation. Nature Physics, 2021, 17, 368-373.	16.7	10
22	Quantitative Waveform Sampling on Atomic Scales. , 2021, , .		0
23	High Harmonics and Isolated Attosecond Pulses from <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline" overflow="scroll"><mml:mrow><mml:mi>Mg</mml:mi><mml:mi mathvariant="normal">O</mml:mi></mml:mrow></mml:math>. Physical Review Applied, 2021, 15, .	3.8	26
24	Higher-Order Band Topology in Twisted MoirÃ© Superlattice. Physical Review Letters, 2021, 126, 066401.	7.8	56
25	MoirÃ© heterostructures as a condensed-matter quantum simulator. Nature Physics, 2021, 17, 155-163.	16.7	317
26	Enhanced tunable second harmonic generation from twistable interfaces and vertical superlattices in boron nitride homostructures. Science Advances, 2021, 7, .	10.3	73
27	Intermolecular interactions in optical cavities: An ab initio QED study. Journal of Chemical Physics, 2021, 154, 094113.	3.0	81
28	Single and double charge transfer in the <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mrow><mml:msup><mml:mrow><mml:mi>Ne</mml:mi></mml:mrow><m collision within time-dependent density-functional theory. Physical Review A, 2021, 103, .	2.5	7
29	Simulating Vibronic Spectra without Bornâ€“Oppenheimer Surfaces. Journal of Physical Chemistry Letters, 2021, 12, 3074-3081.	4.6	8
30	Ultrafast dynamical Lifshitz transition. Science Advances, 2021, 7, .	10.3	38
31	Real-time observation of a correlation-driven sub 3â€‰fs charge migration in ionised adenine. Communications Chemistry, 2021, 4, .	4.5	38
32	Identification of the Mott Insulating Charge Density Wave State in <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:mn>1</mml:mn><mml:mi mathvariant="normal">T</mml:mi><mml:mtext>â€“</mml:mtext><mml:mi>Ta</mml:mi><mml:msub><mml:mrow><mml:mi mathvariant="normal">S</mml:mi></mml:mrow><mml:mrow><mml:mn>2</mml:mn></mml:mrow></mml:msub></mml:mrow></mml:m Physical Review Letters, 2021, 126, 196406.	7.8	27
33	Light-Induced Charge Transfer from Transition-Metal-Doped Aluminum Clusters to Carbon Dioxide. Journal of Physical Chemistry A, 2021, 125, 5878-5885.	2.5	2
34	Phonoritons as Hybridized Exciton-Photon-Phonon Excitations in a Monolayer <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mi>h</mml:mi></mml:math> -BN Optical Cavity. Physical Review Letters, 2021, 126, 227401.	7.8	18
35	Survival of Floquetâ€“Bloch States in the Presence of Scattering. Nano Letters, 2021, 21, 5028-5035.	9.1	41
36	Strong chiral dichroism and enantiopurification in above-threshold ionization with locally chiral light. Physical Review Research, 2021, 3, .	3.6	9

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37	The ferroelectric photo ground state of SrTiO ₃ : Cavity materials engineering. Proceedings of the National Academy of Sciences of the United States of America, 2021, 118, .	7.1	49
38	Down-conversion processes inab initiononrelativistic quantum electrodynamics. Physical Review Research, 2021, 3, .	3.6	8
39	Out-of-Plane Transport of 1T-TaS₂/Graphene-Based van der Waals Heterostructures. ACS Nano, 2021, 15, 11898-11907.	14.6	20
40	Approximations based on density-matrix embedding theory for density-functional theories. Electronic Structure, 2021, 3, 035001.	2.8	1
41	Quantum paraelectric phase of <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:msub><mml:mi>SrTiO</mml:mi><mml:mn>3</mml:mn></mml:msub><mml:msub><mml:mi></mml:mi></mml:msub><mml:mi></mml:mi></mml:math> from first principles. Physical Review B, 2021, 104, .	3.2	22
42	Light-Driven Extremely Nonlinear Bulk Photogalvanic Currents. Physical Review Letters, 2021, 127, 126601.	7.8	25
43	Nematicity Arising from a Chiral Superconducting Ground State in Magic-Angle Twisted Bilayer Graphene under In-Plane Magnetic Fields. Physical Review Letters, 2021, 127, 127001.	7.8	13
44	Engineering Three-Dimensional MoirÃ© Flat Bands. Nano Letters, 2021, 21, 7519-7526.	9.1	10
45	MoirÃ©less correlations in ABCA graphene. Proceedings of the National Academy of Sciences of the United States of America, 2021, 118, .	7.1	59
46	Polaritonic Chemistry: Collective Strong Coupling Implies Strong Local Modification of Chemical Properties. Journal of Physical Chemistry Letters, 2021, 12, 508-516.	4.6	65
47	Realization of nearly dispersionless bands with strong orbital anisotropy from destructive interference in twisted bilayer MoS2. Nature Communications, 2021, 12, 5644.	12.8	57
48	Making ab initio QED functional(s): Nonperturbative and photon-free effective frameworks for strong lightâ€“matter coupling. Proceedings of the National Academy of Sciences of the United States of America, 2021, 118, .	7.1	42
49	Conditional Wave Function Theory: A Unified Treatment of Molecular Structure and Nonadiabatic Dynamics. Journal of Chemical Theory and Computation, 2021, , .	5.3	1
50	Common microscopic origin of the phase transitions in Ta2NiS5 and the excitonic insulator candidate Ta2NiSe5. Npj Computational Materials, 2021, 7, .	8.7	19
51	Photoionization and transient Wannier-Stark ladder in silicon: First-principles simulations versus Keldysh theory. Physical Review B, 2021, 104, .	3.2	7
52	Entangled photon assisted multidimensional nonlinear optics of excitonâ€“polaritons. Journal of Applied Physics, 2020, 128, 113102.	2.5	13
53	How Circular Dichroism in Time- and Angle-Resolved Photoemission Can Be Used to Spectroscopically Detect Transient Topological States in Graphene. Physical Review X, 2020, 10, .	8.9	29
54	Parameter-free hybridlike functional based on an extended Hubbard model: <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mrow><mml:mi>DFT</mml:mi><mml:mo>+</mml:mo><mml:mi>U</mml:mi></mml:mrow></mml:math> Physical Review B, 2020, 102, .	3.2	42

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55	Dynamical amplification of electric polarization through nonlinear phononics in 2D SnTe. Npj Computational Materials, 2020, 6, .	8.7	12
56	Charge-Transfer Plasmon Polaritons at Graphene/Î±-RuCl₃ Interfaces. Nano Letters, 2020, 20, 8438-8445.	9.1	53
57	Lightâ€“Matter Hybrid-Orbital-Based First-Principles Methods: The Influence of Polariton Statistics. Journal of Chemical Theory and Computation, 2020, 16, 5601-5620.	5.3	19
58	Exact exchange-correlation potential of effectively interacting Kohn-Sham systems. Physical Review A, 2020, 101, .	2.5	1
59	Effect of many modes on self-polarization and photochemical suppression in cavities. Journal of Chemical Physics, 2020, 153, 104103.	3.0	44
60	Direct Measurement of Electron-Phonon Coupling with Time-Resolved ARPES. Physical Review Letters, 2020, 125, 136401.	7.8	27
61	Virial Relations for Electrons Coupled to Quantum Field Modes. Journal of Chemical Theory and Computation, 2020, 16, 6236-6243.	5.3	6
62	Chemistry in Quantum Cavities: Exact Results, the Impact of Thermal Velocities, and Modified Dissociation. Journal of Physical Chemistry Letters, 2020, 11, 7525-7530.	4.6	26
63	Giant Exciton Mott Density in Anatase <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:msub><mml:mrow><mml:mi>TiO</mml:mi></mml:mrow><mml:mrow><mml:mn>2</mml:mn></mml:mrow></mml:msub></mml:mrow></mml:math> Physical Review Letters, 2020, 125, 116403.	7.8	8
64	Coupled Cluster Theory for Molecular Polaritons: Changing Ground and Excited States. Physical Review X, 2020, 10, .	8.9	102
65	Ultrafast transient absorption spectroscopy of the charge-transfer insulator NiO: Beyond the dynamical Franz-Keldysh effect. Physical Review B, 2020, 102, .	3.2	12
66	Nature of Symmetry Breaking at the Excitonic Insulator Transition: <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:msub><mml:mrow><mml:mi>Ta</mml:mi></mml:mrow><mml:mrow><mml:mn>2</mml:mn></mml:mrow></mml:msub></mml:mrow></mml:math> Physical Review Letters, 2020, 124, 197601.	7.8	73
67	Correlated electronic phases in twisted bilayer transition metal dichalcogenides. Nature Materials, 2020, 19, 861-866.	27.5	544
68	Room Temperature Terahertz Electroabsorption Modulation by Excitons in Monolayer Transition Metal Dichalcogenides. Nano Letters, 2020, 20, 5214-5220.	9.1	14
69	Polycyclic aromatic chains on metals and insulating layers by repetitive [3+2]Âcycloadditions. Nature Communications, 2020, 11, 1490.	12.8	23
70	Electronâ€“phonon-driven three-dimensional metallicity in an insulating cuprate. Proceedings of the National Academy of Sciences of the United States of America, 2020, 117, 6409-6416.	7.1	18
71	Octopus, a computational framework for exploring light-driven phenomena and quantum dynamics in extended and finite systems. Journal of Chemical Physics, 2020, 152, 124119.	3.0	210
72	Local Berry curvature signatures in dichroic angle-resolved photoelectron spectroscopy from two-dimensional materials. Science Advances, 2020, 6, eaay2730.	10.3	57

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73	Setting the photoelectron clock through molecular alignment. Nature Communications, 2020, 11, 2546.	12.8	26
74	Universal slow plasmons and giant field enhancement in atomically thin quasi-two-dimensional metals. Nature Communications, 2020, 11, 1013.	12.8	53
75	Relevance of the Quadratic Diamagnetic and Self-Polarization Terms in Cavity Quantum Electrodynamics. ACS Photonics, 2020, 7, 975-990.	6.6	105
76	Covalent Câ€“N Bond Formation through a Surface Catalyzed Thermal Cyclodehydrogenation. Journal of the American Chemical Society, 2020, 142, 3696-3700.	13.7	27
77	High-harmonic generation from spin-polarised defects in solids. Npj Computational Materials, 2020, 6, .	8.7	48
78	Polaritonic coupled-cluster theory. Physical Review Research, 2020, 2, .	3.6	57
79	Polariton panorama. Nanophotonics, 2020, 10, 549-577.	6.0	155
80	Light-induced topological magnons in two-dimensional van der Waals magnets. SciPost Physics, 2020, 9, .	4.9	18
81	Role of electron scattering on the high-order harmonic generation from solids. Physical Review Research, 2020, 2, .	3.6	3
82	Electronic Structure of Materials by Ab Initio Methods: Overview. , 2020, , 207-212.		0
83	Quantum Electrodynamical Bloch Theory with Homogeneous Magnetic Fields. Physical Review Letters, 2019, 123, 047202.	7.8	30
84	Maximized electron interactions at the magic angle in twisted bilayer graphene. Nature, 2019, 572, 95-100.	27.8	644
85	Multiflat Bands and Strong Correlations in Twisted Bilayer Boron Nitride: Doping-Induced Correlated Insulator and Superconductor. Nano Letters, 2019, 19, 4934-4940.	9.1	123
86	Integration of CLIP experiments of RNA-binding proteins: a novel approach to predict context-dependent splicing factors from transcriptomic data. BMC Genomics, 2019, 20, 521.	2.8	4
87	Force balance approach for advanced approximations in density functional theories. Journal of Chemical Physics, 2019, 151, 154107.	3.0	17
88	Self-Consistent Density-Functional Embedding: A Novel Approach for Density-Functional Approximations. Journal of Chemical Theory and Computation, 2019, 15, 5209-5220.	5.3	14
89	Reduced Density-Matrix Approach to Strong Matter-Photon Interaction. ACS Photonics, 2019, 6, 2694-2711.	6.6	31
90	Lightâ€“Matter Response in Nonrelativistic Quantum Electrodynamics. ACS Photonics, 2019, 6, 2757-2778.	6.6	79

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91	Capturing vacuum fluctuations and photon correlations in cavity quantum electrodynamics with multitrajectory Ehrenfest dynamics. Physical Review A, 2019, 99, .	2.5	33
92	Cavity Control of Excitons in Two-Dimensional Materials. Nano Letters, 2019, 19, 3473-3479.	9.1	65
93	Density-Matrix Embedding Theory Study of the One-Dimensional Hubbardâ€“Holstein Model. Journal of Chemical Theory and Computation, 2019, 15, 2221-2232.	5.3	22
94	Orbital magneto-optical response of periodic insulators from first principles. Npj Computational Materials, 2019, 5, .	8.7	5
95	Modification of excitation and charge transfer in cavity quantum-electrodynamical chemistry. Proceedings of the National Academy of Sciences of the United States of America, 2019, 116, 4883-4892.	7.1	138
96	Unraveling materials Berry curvature and Chern numbers from real-time evolution of Bloch states. Proceedings of the National Academy of Sciences of the United States of America, 2019, 116, 4135-4140.	7.1	20
97	Light-matter interactions within the Ehrenfestâ€“Maxwellâ€“Pauliâ€“Kohnâ€“Sham framework: fundamentals, implementation, and nano-optical applications. Advances in Physics, 2019, 68, 225-333.	14.4	54
98	Attosecond Electron Localization and Screening Dynamics in Metals. , 2019, , .		0
99	Exciton control in a room temperature bulk semiconductor with coherent strain pulses. Science Advances, 2019, 5, eaax2937.	10.3	28
100	Benchmarking semiclassical and perturbative methods for real-time simulations of cavity-bound emission and interference. Journal of Chemical Physics, 2019, 151, 244113.	3.0	37
101	Optimal control theory for quantum electrodynamics: an initial state problem. European Physical Journal B, 2019, 92, 1.	1.5	6
102	Upstream analysis of alternative splicing: a review of computational approaches to predict context-dependent splicing factors. Briefings in Bioinformatics, 2019, 20, 1358-1375.	6.5	53
103	Nonadiabatic quantum dynamics without potential energy surfaces. Physical Review Materials, 2019, 3, .	2.4	12
104	Topological Floquet engineering of twisted bilayer graphene. Physical Review Research, 2019, 1, .	3.6	56
105	Electronic Structure of Materials by Ab Initio Methods: Overview. , 2019, , 1-6.		0
106	From a quantum-electrodynamical lightâ€“matter description to novel spectroscopies. Nature Reviews Chemistry, 2018, 2, .	30.2	182
107	Ab Initio Optimized Effective Potentials for Real Molecules in Optical Cavities: Photon Contributions to the Molecular Ground State. ACS Photonics, 2018, 5, 992-1005.	6.6	96
108	Propagators for the Time-Dependent Kohnâ€“Sham Equations: Multistep, Rungeâ€“Kutta, Exponential Rungeâ€“Kutta, and Commutator Free Magnus Methods. Journal of Chemical Theory and Computation, 2018, 14, 3040-3052.	5.3	69

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109	Atomic-like high-harmonic generation from two-dimensional materials. Science Advances, 2018, 4, eaao5207.	10.3	98
110	Phonon-driven spin-Floquet magneto-valleytronics in MoS2. Nature Communications, 2018, 9, 638.	12.8	86
111	Phonon Driven Floquet Matter. Nano Letters, 2018, 18, 1535-1542.	9.1	63
112	Lightâ€“matter interaction in the long-wavelength limit: no ground-state without dipole self-energy. Journal of Physics B: Atomic, Molecular and Optical Physics, 2018, 51, 034005.	1.5	132
113	Ab Initio Simulation of Attosecond Transient Absorption Spectroscopy in Two-Dimensional Materials. Applied Sciences (Switzerland), 2018, 8, 1777.	2.5	19
114	All-optical nonequilibrium pathway to stabilising magnetic Weyl semimetals in pyrochlore iridates. Nature Communications, 2018, 9, 4452.	12.8	38
115	Electronic Structure of Materials by Ab Initio Methods: Overview. , 2018, , 1-6.		1
116	Atomic and Electronic Structure of Silicene on Ag: A Theoretical Perspective. Nanoscience and Technology, 2018, , 159-178.	1.5	1
117	Special issue in honor of Eberhard K.U. Gross for his 65th birthday. European Physical Journal B, 2018, 91, 1.	1.5	0
118	Ab initiononrelativistic quantum electrodynamics: Bridging quantum chemistry and quantum optics from weak to strong coupling. Physical Review A, 2018, 98, .	2.5	126
119	Multiple-orbital effects in laser-induced electron diffraction of aligned molecules. Physical Review A, 2018, 98, .	2.5	14
120	Comparison of RNA-seq and microarray platforms for splice event detection using a cross-platform algorithm. BMC Genomics, 2018, 19, 703.	2.8	20
121	High-harmonic generation from few-layer hexagonal boron nitride: Evolution from monolayer to bulk response. Physical Review B, 2018, 98, .	3.2	54
122	Ultrafast Modification of Hubbard<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:mi>U</mml:mi></mml:mrow></mml:math>in a Strongly Correlated Material:AbÂinitioHigh-Harmonic Generation in NiO. Physical Review Letters, 2018, 121, 097402.	7.8	118
123	Coupled forward-backward trajectory approach for nonequilibrium electron-ion dynamics. Physical Review B, 2018, 97, .	3.2	12
124	Role of intraband transitions in photocarrier generation. Physical Review B, 2018, 98, .	3.2	26
125	Phonon-Driven Selective Modulation of Exciton Oscillator Strengths in Anatase TiO₂ Nanoparticles. Nano Letters, 2018, 18, 5007-5014.	9.1	29
126	Kinetic-Energy Density-Functional Theory on a Lattice. Journal of Chemical Theory and Computation, 2018, 14, 4072-4087.	5.3	7

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127	First-principles simulations for attosecond photoelectron spectroscopy based on time-dependent density functional theory. European Physical Journal B, 2018, 91, 1.	1.5	15
128	Electronic Structure of Materials by Ab Initio Methods: Overview. , 2018, , 1-6.		0
129	Light-matter interactions via the exact factorization approach. European Physical Journal B, 2018, 91, 1.	1.5	44
130	A 400,000-year-old Acheulean assemblage associated with the Aroeira-3 human cranium (Gruta da) Tj ETQq0 0 0 rgBT /Overlock 10 Tf 50	0.2	20
131	Emergent elemental two-dimensional materials beyond graphene. Journal Physics D: Applied Physics, 2017, 50, 053004.	2.8	74
132	Creating stable Floquetâ€“Weyl semimetals by laser-driving of 3D Dirac materials. Nature Communications, 2017, 8, 13940.	12.8	255
133	Ab initio Modelling of Plasmons in Metalâ€semiconductor Bilayer Transitionâ€metal Dichalcogenide Heterostructures. Israel Journal of Chemistry, 2017, 57, 540-546.	2.3	4
134	Atoms and molecules in cavities, from weak to strong coupling in quantum-electrodynamics (QED) chemistry. Proceedings of the National Academy of Sciences of the United States of America, 2017, 114, 3026-3034.	7.1	389
135	Impact of the Electronic Band Structure in High-Harmonic Generation Spectra of Solids. Physical Review Letters, 2017, 118, 087403.	7.8	226
136	Efficient and accurate modeling of electron photoemission in nanostructures with TDDFT. European Physical Journal B, 2017, 90, 1.	1.5	32
137	New Middle Pleistocene hominin cranium from Gruta da Aroeira (Portugal). Proceedings of the National Academy of Sciences of the United States of America, 2017, 114, 3397-3402.	7.1	81
138	Cavity Bornâ€“Oppenheimer Approximation for Correlated Electronâ€“Nuclear-Photon Systems. Journal of Chemical Theory and Computation, 2017, 13, 1616-1625.	5.3	133
139	A First-Principles Time-Dependent Density Functional Theory Framework for Spin and Time-Resolved Angular-Resolved Photoelectron Spectroscopy in Periodic Systems. Journal of Chemical Theory and Computation, 2017, 13, 265-273.	5.3	49
140	Ellipticity dependence of high-harmonic generation in solids originating from coupled intraband and interband dynamics. Nature Communications, 2017, 8, 745.	12.8	146
141	Modeling of laser-pulse induced water decomposition on two-dimensional materials by simulations based on time-dependent density functional theory. Physical Review B, 2017, 96, .	3.2	20
142	Anomalous anisotropic exciton temperature dependence in rutile <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:msub><mml:mi>TiO</mml:mi><mml:mn>2</mml:mn></mml:msub></mml Physical Review B, 2017, 96, .	3.2	8
143	TDDFT-Based Study on the Protonâ€“DNA Collision. Journal of Physical Chemistry B, 2017, 121, 7276-7283.	2.6	8
144	Introduction to the Physics of Silicene and other 2D Materials. Lecture Notes in Physics, 2017, , .	0.7	33

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145	A Brief History of Silicene. Lecture Notes in Physics, 2017, , 1-11.	0.7	0
146	Freestanding Silicene. Lecture Notes in Physics, 2017, , 13-39.	0.7	3
147	Multilayer Silicene. Lecture Notes in Physics, 2017, , 53-61.	0.7	0
148	Germanene, Stanene and Other 2D Materials. Lecture Notes in Physics, 2017, , 63-85.	0.7	4
149	Bimodal supramolecular functionalization of carbon nanotubes triggered by covalent bond formation. Chemical Science, 2017, 8, 1927-1935.	7.4	29
150	Self-consistent <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mi mathvariant="normal">DFT</mml:mi><mml:mo>+</mml:mo><mml:mi>U</mml:mi></mml:math> method for real-space time-dependent density functional theory calculations. Physical Review B, 2017, 96, .	3.2	35
151	Exact functionals for correlated electronâ€“photon systems. New Journal of Physics, 2017, 19, 113036.	2.9	19
152	Electronic band gaps of confined linear carbon chains ranging from polyyne to carbyne. Physical Review Materials, 2017, 1, .	2.4	61
153	Exact maps in density functional theory for lattice models. New Journal of Physics, 2016, 18, 083004.	2.9	13
154	Universal steps in quantum dynamics with time-dependent potential-energy surfaces: Beyond the Born-Oppenheimer picture. Physical Review A, 2016, 94, .	2.5	10
155	Negative plasmon dispersion in 2H-NbS₂beyond the charge-density-wave interpretation. New Journal of Physics, 2016, 18, 103050.	2.9	10
156	Tailored pump-probe transient spectroscopy with time-dependent density-functional theory: controlling absorption spectra. European Physical Journal B, 2016, 89, 1.	1.5	17
157	Confined linear carbon chains as a route to bulkÂcarbyne. Nature Materials, 2016, 15, 634-639.	27.5	341
158	The mechanical bond on carbon nanotubes: diameter-selective functionalization and effects on physical properties. Nanoscale, 2016, 8, 9254-9264.	5.6	33
159	Imaging single-molecule reaction intermediates stabilized by surface dissipation and entropy. Nature Chemistry, 2016, 8, 678-683.	13.6	130
160	Disentangling Vacancy Oxidation on Metallicity-Sorted Carbon Nanotubes. Journal of Physical Chemistry C, 2016, 120, 18316-18322.	3.1	8
161	Noncovalent Dimerization after Enediyne Cyclization on Au(111). Journal of the American Chemical Society, 2016, 138, 10963-10967.	13.7	15
162	Stability of the Dirac cone in artificial graphene formed in quantum wells: a computational many-electron study. New Journal of Physics, 2016, 18, 083014.	2.9	7

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163	A largeâ€scale analysis of alternative splicing reveals a key role of QKI in lung cancer. Molecular Oncology, 2016, 10, 1437-1449.	4.6	60
164	Monitoring Electron-Photon Dressing in WSe₂. Nano Letters, 2016, 16, 7993-7998.	9.1	64
165	Density functional theory study of theÎ±â^Î³phase transition in cerium: Role of electron correlation andf-orbital localization. Physical Review B, 2016, 93, .	3.2	23
166	Polyyne electronic and vibrational properties under environmental interactions. Physical Review B, 2016, 94, .	3.2	45
167	Systematic construction of density functionals based on matrix product state computations. New Journal of Physics, 2016, 18, 083039.	2.9	16
168	On the Exciton Coupling between Two Chlorophyll Pigments in the Absence of a Protein Environment: Intrinsic Effects Revealed by Theory and Experiment. Angewandte Chemie, 2016, 128, 6356-6359.	2.0	4
169	Quantum plasmonics: from jellium models to ab initio calculations. Nanophotonics, 2016, 5, 409-426.	6.0	116
170	Electronic Structure of Low-Dimensional Carbon Ï€-Systems. Journal of Physical Chemistry C, 2016, 120, 12362-12368.	3.1	0
171	On the Exciton Coupling between Two Chlorophyll Pigments in the Absence of a Protein Environment: Intrinsic Effects Revealed by Theory and Experiment. Angewandte Chemie - International Edition, 2016, 55, 6248-6251.	13.8	19
172	Photoinduced Absorption within Single-Walled Carbon Nanotube Systems. Journal of Physical Chemistry C, 2016, 120, 1926-1935.	3.1	12
173	Static correlation and electron localization in molecular dimers from the self-consistent RPA and<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></mm Physical Review B, 2015, 91, .	3.2	54
174	Optimized Effective Potential for Quantum Electrodynamical Time-Dependent Density Functional Theory. Physical Review Letters, 2015, 115, 093001.	7.8	93
175	Engineering Photophenomena in Large, 3D Structures Composed of Selfâ€Assembled van der Waals Heterostructure Flakes. Advanced Optical Materials, 2015, 3, 1551-1556.	7.3	17
176	Emergent photophenomena in three dimensional van der Waals heterostructures. , 2015, , .		0
177	Effect of a Single Water Molecule on the Electronic Absorption by o- and p-Nitrophenolate: A Shift to the Red or to the Blue?. Journal of Physical Chemistry A, 2015, 119, 11498-11503.	2.5	13
178	Kohnâ€“Sham approach to quantum electrodynamical density-functional theory: Exact time-dependent effective potentials in real space. Proceedings of the National Academy of Sciences of the United States of America, 2015, 112, 15285-15290.	7.1	107
179	Exciton dispersion in molecular solids. Journal of Physics Condensed Matter, 2015, 27, 113204.	1.8	74
180	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

#	Article	IF	Citations
181	Insights into colour-tuning of chlorophyll optical response in green plants. Physical Chemistry Chemical Physics, 2015, 17, 26599-26606.	2.8	46
182	Optimal thermoelectric figure of merit of Si/Ge core-shell nanowires. Nano Research, 2015, 8, 2611-2619.	10.4	19
183	Comparing Quasiparticle H₂O Level Alignment on Anatase and Rutile TiO₂. ACS Catalysis, 2015, 5, 4242-4254.	11.2	50
184	Modifying the Interlayer Interaction in Layered Materials with an Intense IR Laser. Physical Review Letters, 2015, 114, 116102.	7.8	22
185	The Soret absorption band of isolated chlorophyll a and b tagged with quaternary ammonium ions. Physical Chemistry Chemical Physics, 2015, 17, 25793-25798.	2.8	41
186	Dynamical Processes in Open Quantum Systems from a TDDFT Perspective: Resonances and Electron Photoemission. Topics in Current Chemistry, 2015, 368, 219-271.	4.0	3
187	Modeling electron dynamics coupled to continuum states in finite volumes with absorbing boundaries. European Physical Journal B, 2015, 88, 1.	1.5	64
188	Real-space grids and the Octopus code as tools for the development of new simulation approaches for electronic systems. Physical Chemistry Chemical Physics, 2015, 17, 31371-31396.	2.8	376
189	Design of two-photon molecular tandem architectures for solar cells by ab initio theory. Chemical Science, 2015, 6, 3018-3025.	7.4	9
190	Conditional Bornâ€“Oppenheimer Dynamics: Quantum Dynamics Simulations for the Model Porphine. Journal of Physical Chemistry Letters, 2015, 6, 1529-1535.	4.6	21
191	Anisotropy Effects on the Plasmonic Response of Nanoparticle Dimers. Journal of Physical Chemistry Letters, 2015, 6, 1891-1898.	4.6	30
192	Unraveling the Intrinsic Color of Chlorophyll. Angewandte Chemie - International Edition, 2015, 54, 2170-2173.	13.8	55
193	Optical field terahertz amplitude modulation by graphene nanoribbons. Nanoscale, 2015, 7, 19012-19017.	5.6	6
194	Orbitals from local RDMFT: Are they Kohn-Sham or natural orbitals?. Journal of Chemical Physics, 2015, 143, 054106.	3.0	10
195	Advances in network-based metabolic pathway analysis and gene expression data integration. Briefings in Bioinformatics, 2015, 16, 265-279.	6.5	25
196	In-Silico Prediction of Key Metabolic Differences between Two Non-Small Cell Lung Cancer Subtypes. PLoS ONE, 2014, 9, e103998.	2.5	25
197	Identification of structural motifs as tunneling two-level systems in amorphous alumina at low temperatures. Physical Review B, 2014, 90, .	3.2	21
198	Energyâ€transfer in porphyrinâ€•functionalized graphene. Physica Status Solidi (B): Basic Research, 2014, 251, 2495-2498.	1.5	2

#	Article	IF	Citations
199	Coherent ultrafast charge transfer in an organic photovoltaic blend. , 2014, , .		0
200	Local reduced-density-matrix-functional theory: Incorporating static correlation effects in Kohn-Sham equations. Physical Review A, 2014, 90, .	2.5	32
201	Photo-induced strengthening of weak bonding in noble gas dimers. Applied Physics Letters, 2014, 104, 201107.	3.3	2
202	Recent Memory and Performance Improvements in Octopus Code. Lecture Notes in Computer Science, 2014, , 607-622.	1.3	3
203	Ab initionanoplasmonics: The impact of atomic structure. Physical Review B, 2014, 90, .	3.2	147
204	Interplay between structure and electronic properties of layered transition-metal dichalcogenides: Comparing the loss function of<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mrow><mml:mn>1</mml:mn><mml:mi>T</mml:mi></mml:mrow></mml:m<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mrow><mml:mn>2</mml:mn><mml:mi>H</mml:mi></mml:mrow></mml:m Physical Review B, 2014, 90, .	3.2	18
205	Quasi-particle energy spectra in local reduced density matrix functional theory. Journal of Chemical Physics, 2014, 141, 164120.	3.0	15
206	Crossâ€Conjugation vs. Linear Conjugation in Donorâ€“Bridgeâ€“Acceptor Nitrophenol Chromophores. European Journal of Organic Chemistry, 2014, 2014, 2044-2052.	2.4	8
207	Mechanically Interlocked Singleâ€Wall Carbon Nanotubes. Angewandte Chemie - International Edition, 2014, 53, 5394-5400.	13.8	69
208	Coherent ultrafast charge transfer in an organic photovoltaic blend. Science, 2014, 344, 1001-1005.	12.6	470
209	Instantaneous Band Gap Collapse in Photoexcited Monoclinic<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:msub><mml:mrow><mml:mi>VO</mml:mi></mml:mrow><mml:mrow><mml:mn>2</mml:mn></ to Photocarrier Doping. Physical Review Letters, 2014, 113, 216401.	7.8	203
210	Silicite: The layered allotrope of silicon. Physical Review B, 2014, 90, .	3.2	59
211	High-energy collective electronic excitations in layered transition-metal dichalcogenides. Physical Review B, 2014, 90, .	3.2	15
212	First-principles description of charge transfer in donor-acceptor compounds from self-consistent many-body perturbation theory. Physical Review B, 2014, 90, .	3.2	44
213	A survey of the parallel performance and accuracy of Poisson solvers for electronic structure calculations. Journal of Computational Chemistry, 2014, 35, 427-444.	3.3	23
214	Correlated Electron-Nuclear Dynamics with Conditional Wave Functions. Physical Review Letters, 2014, 113, 083003.	7.8	30
215	Identification of Alternative Splicing Events Regulated by the Oncogenic Factor SRSF1 in Lung Cancer. Cancer Research, 2014, 74, 1105-1115.	0.9	77
216	Photoinduced Câ€“C Reactions on Insulators toward Photolithography of Graphene Nanoarchitectures. Journal of the American Chemical Society, 2014, 136, 4651-4658.	13.7	45

#	Article	IF	Citations
217	Spectroscopy of Nitrophenolates in Vacuo: Effect of Spacer, Configuration, and Microsolvation on the Charge-Transfer Excitation Energy. Accounts of Chemical Research, 2014, 47, 1417-1425.	15.6	21
218	Quasiparticle Level Alignment for Photocatalytic Interfaces. Journal of Chemical Theory and Computation, 2014, 10, 2103-2113.	5.3	60
219	Quantum-electrodynamical density-functional theory: Bridging quantum optics and electronic-structure theory. Physical Review A, 2014, 90, .	2.5	197
220	FÃ¶rster-Induced Energy Transfer in Functionalized Graphene. Journal of Physical Chemistry C, 2014, 118, 9283-9289.	3.1	32
221	Revealing the Adsorption Mechanisms of Nitroxides on Ultrapure, Metallicity-Sorted Carbon Nanotubes. ACS Nano, 2014, 8, 1375-1383.	14.6	31
222	Nonadiabatic and Time-Resolved Photoelectron Spectroscopy for Molecular Systems. Journal of Chemical Theory and Computation, 2014, 10, 1665-1676.	5.3	7
223	PFOâ€“BPy solubilizers for SWNTs: Modelling of polymers from oligomers. Physica Status Solidi (B): Basic Research, 2014, 251, 2407-2412.	1.5	6
224	Level Alignment of a Prototypical Photocatalytic System: Methanol on TiO₂(110). Journal of the American Chemical Society, 2013, 135, 11429-11432.	13.7	68
225	Metallicity retained by covalent functionalization of graphene with phenyl groups. Nanoscale, 2013, 5, 7537.	5.6	9
226	Understanding Energy-Level Alignment in Donorâ€“Acceptor/Metal Interfaces from Core-Level Shifts. ACS Nano, 2013, 7, 6914-6920.	14.6	78
227	Frenkel versus charge-transfer exciton dispersion in molecular crystals. Physical Review B, 2013, 88, .	3.2	49
228	Solvent-mediated folding of dicarboxylate dianions: aliphatic chain length dependence and origin of the IR intensity quenching. Physical Chemistry Chemical Physics, 2013, 15, 20463.	2.8	8
229	A proposed family of variationally correlated first-order density matrices for spin-polarized three-electron model atoms. Journal of Mathematical Chemistry, 2013, 51, 763-773.	1.5	0
230	Correlation effects in the optical spectra of porphyrin oligomer chains: Exciton confinement and length dependence. Journal of Chemical Physics, 2013, 138, 024312.	3.0	31
231	Self-consistent<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:mi>G</mml:mi><mml:mi>W</mml:mi></mml:mrow></mml:math>: All-electron implementation with localized basis functions. Physical Review B, 2013, 88, .	3.2	135
232	Quantum coherence controls the charge separation in a prototypical artificial light-harvesting system. Nature Communications, 2013, 4, 1602.	12.8	239
233	Simulating Pumpâ€“Probe Photoelectron and Absorption Spectroscopy on the Attosecond Timescale with Timeâ€Dependent Density Functional Theory. ChemPhysChem, 2013, 14, 1363-1376.	2.1	87
234	Performance of Nonlocal Optics When Applied to Plasmonic Nanostructures. Journal of Physical Chemistry C, 2013, 117, 8941-8949.	3.1	103

#	Article	IF	Citations
235	Bond Breaking and Bond Formation: How Electron Correlation is Captured in Many-Body Perturbation Theory and Density-Functional Theory. Physical Review Letters, 2013, 110, 146403.	7.8	82
236	Direct Imaging of Covalent Bond Structure in Single-Molecule Chemical Reactions. Science, 2013, 340, 1434-1437.	12.6	513
237	On the Effect of a Single Solvent Molecule on the Charge-Transfer Band of a Donorâ€“Acceptor Anion. Journal of the American Chemical Society, 2013, 135, 6818-6821.	13.7	21
238	Electronic structure of Fe- vs. Ru-based dye molecules. Journal of Chemical Physics, 2013, 138, 044709.	3.0	13
239	Stark Ionization of Atoms and Molecules within Density Functional Resonance Theory. Journal of Physical Chemistry Letters, 2013, 4, 2734-2738.	4.6	18
240	Influence of Axial and Peripheral Ligands on the Electronic Structure of Titanium Phthalocyanines. Journal of Physical Chemistry C, 2013, 117, 4410-4420.	3.1	24
241	Efficient Gate-tunable light-emitting device made of defective boron nitride nanotubes: from ultraviolet to the visible. Scientific Reports, 2013, 3, 2698.	3.3	22
242	Long-lived oscillatory incoherent electron dynamics in molecules:trans-polyacetylene oligomers. New Journal of Physics, 2013, 15, 043004.	2.9	11
243	Selection of human tissue-specific elementary flux modes using gene expression data. Bioinformatics, 2013, 29, 2009-2016.	4.1	38
244	Local-field effects on the plasmon dispersion of two-dimensional transition metal dichalcogenides. New Journal of Physics, 2013, 15, 125005.	2.9	18
245	Loss spectroscopy of molecular solids: combining experiment and theory. New Journal of Physics, 2013, 15, 125024.	2.9	15
246	The Isolation of Single MMX Chains from Solution: Unravelling the Assemblyâ€“Disassembly Process. Chemistry - A European Journal, 2013, 19, 15518-15529.	3.3	7
247	Theoretical Methods. Physical Chemistry in Action, 2013, , 45-65.	0.6	0
248	Enhanced thermoelectric properties in hybrid graphene/boron nitride nanoribbons. Physical Review B, 2012, 86, .	3.2	138
249	Role of nonlocal exchange in the electronic structure of correlated oxides. Physical Review B, 2012, 85, .	3.2	65
250	Plasmon dispersion in layered transition-metal dichalcogenides. Physical Review B, 2012, 86, .	3.2	45
251	Density-Functional Theory for<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mi>f</mml:mi></mml:math>-Electron Systems: The<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mi>Î±</mml:mi><mml:mtext mathvariant="normal">â^'</mml:mtext><mml:mi>Î³</mml:mi></mml:math>Phase Transition in Cerium. Physical Review Letters, 2012, 109, 146402.	7.8	62
252	Pulse-induced nonequilibrium dynamics of acetylene inside carbon nanotube studied by an ab initio approach. Proceedings of the National Academy of Sciences of the United States of America, 2012, 109, 8861-8865.	7.1	4

#	Article	IF	Citations
253	Response Functions in TDDFT: Concepts and Implementation. Lecture Notes in Physics, 2012, , 139-166.	0.7	14
254	Anomalous insulator-metal transition in boron nitride-graphene hybrid atomic layers. Physical Review B, 2012, 86, .	3.2	42
255	Excitons in molecular crystals from first-principles many-body perturbation theory: Picene versus pentacene. Physical Review B, 2012, 86, .	3.2	99
256	Structural and Optoelectronic Properties of Unsaturated ZnO and ZnS Nanoclusters. Journal of Physical Chemistry C, 2012, 116, 8741-8746.	3.1	41
257	Supramolecular Environment-Dependent Electronic Properties of Metalâ€“Organic Interfaces.. Journal of Physical Chemistry C, 2012, 116, 4780-4785.	3.1	25
258	The Nature of Radiative Transitions in TiO2-Based Nanosheets. Journal of Physical Chemistry C, 2012, 116, 18495-18503.	3.1	31
259	Substitution effects on the absorption spectra of nitrophenolate isomers. Physical Chemistry Chemical Physics, 2012, 14, 12905.	2.8	27
260	Supramolecular Assembly of Diplatinum Species through Weak Pt^{II}â‹…â‹…â‹…Pt^{II} Intermolecular Interactions: A Combined Experimental and Computational Study. Chemistry - A European Journal, 2012, 18, 13787-13799.	3.3	15
261	Electronic and magnetic properties of NiS2, NiSSe and NiSe2 by a combination of theoretical methods. European Physical Journal B, 2012, 85, 1.	1.5	45
262	Benchmark of<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:mi>G</mml:mi><mml:mi>W</mml:mi></mml:mrow></mml:math>methods for azabenzenes. Physical Review B, 2012, 86, .	3.2	154
263	Excited states of the green fluorescent protein chromophore: Performance of ab initio and semiâ€empirical methods. Physica Status Solidi (B): Basic Research, 2012, 249, 392-400.	1.5	32
264	Laser-induced preferential dehydrogenation of graphane. Physical Review B, 2012, 85, .	3.2	13
265	Time-dependent density-functional theory in massively parallel computer architectures: the octopus project. Journal of Physics Condensed Matter, 2012, 24, 233202.	1.8	181
266	Artificially Stacked Atomic Layers: Toward New van der Waals Solids. Nano Letters, 2012, 12, 3518-3525.	9.1	211
267	Four electrons interacting pairwise in the limit of infinitesimal confining potentials: Especially the quintet spin state. Chemical Physics Letters, 2012, 536, 162-164.	2.6	2
268	On the intrinsic optical absorptions by tetrathiafulvalene radical cations and isomers. Chemical Communications, 2011, 47, 6900.	4.1	26
269	Dielectric screening in two-dimensional insulators: Implications for excitonic and impurity states in graphane. Physical Review B, 2011, 84, .	3.2	476
270	Structure, electronic, and optical properties of TiO2 atomic clusters: An ab initio study. Journal of Chemical Physics, 2011, 135, 244704.	3.0	64

#	Article	IF	Citations
271	Spectroscopic Characterization of Solventâ€Mediated Folding in Dicarboxylate Dianions. Angewandte Chemie - International Edition, 2011, 50, 3807-3810.	13.8	17
272	Plasmon dispersion in molecular solids: Picene and potassium-doped picene. Physical Review B, 2011, 84, .	3.2	28
273	Tailoring Electronic and Optical Properties of TiO₂: Nanostructuring, Doping and Molecular-Oxide Interactions. , 2011, , 301-329.		2
274	Charge transfer in time-dependent density-functional theory via spin-symmetry breaking. Physical Review A, 2011, 83, .	2.5	30
275	Unoccupied states in Cu and Zn octaethyl-porphyrin and phthalocyanine. Journal of Chemical Physics, 2011, 134, 204707.	3.0	33
276	Basis set effects on the hyperpolarizability of CHCl3: Gaussian-type orbitals, numerical basis sets and real-space grids. Journal of Chemical Physics, 2010, 133, 034111.	3.0	46
277	Self-energy and excitonic effects in the electronic and optical properties of<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:msub><mml:mrow><mml:mtext>TiO</mml:mtext></mml:mrow><mml:mn>2</mml:mn></mml:msub></mml:mrow></mml:math> phases. Physical Review B, 2010, 82, .	3.2	236
278	Development of a novel splice array platform and its application in the identification of alternative splice variants in lung cancer. BMC Genomics, 2010, 11, 352.	2.8	25
279	Doubleâ€Bond versus Tripleâ€Bond Bridges: Does it Matter for the Chargeâ€Transfer Absorption by Donorâ€“Acceptor Chromophores?. ChemPhysChem, 2010, 11, 2495-2498.	2.1	15
280	Nanoscale patchworks. Nature Materials, 2010, 9, 379-380.	27.5	65
281	Electronic properties of molecular solids: the peculiar case of solid picene. New Journal of Physics, 2010, 12, 103036.	2.9	46
282	Many-Body Effects in the Excitation Spectrum of a Defect in SiC. Physical Review Letters, 2010, 105, 026401.	7.8	66
283	Sodium: A Charge-Transfer Insulator at High Pressures. Physical Review Letters, 2010, 104, 216404.	7.8	61
284	Time-dependent density functional approach for the calculation of inelastic x-ray scattering spectra of molecules. Journal of Chemical Physics, 2010, 133, 174111.	3.0	23
285	The physical and chemical properties of heteronanotubes. Reviews of Modern Physics, 2010, 82, 1843-1885.	45.6	239
286	First-Principles Simulations of Chemical Reactions in an HCl Molecule Embedded inside a C or BN Nanotube Induced by Ultrafast Laser Pulses. Physical Review Letters, 2010, 105, 248301.	7.8	16
287	Strong Charge-Transfer Excitonic Effects and the Bose-Einstein Exciton Condensate in Graphane. Physical Review Letters, 2010, 104, 226804.	7.8	180
288	Photoabsorption spectra of small cationic xenon clusters from time-dependent density functional theory. Journal of Chemical Physics, 2009, 131, 214302.	3.0	4

#	Article	IF	Citations
289	Computing the shortest elementary flux modes in genome-scale metabolic networks. Bioinformatics, 2009, 25, 3158-3165.	4.1	184
290	Customized Electronic Coupling in Selfâ€Assembled Donorâ€“Acceptor Nanostructures. Advanced Functional Materials, 2009, 19, 3567-3573.	14.9	52
291	Absorption Spectra of 4â€Nitrophenolate Ions Measured in Vacuo and in Solution. ChemPhysChem, 2009, 10, 1207-1209.	2.1	29
292	The challenge of predicting optical properties of biomolecules: What can we learn from time-dependent density-functional theory?. Comptes Rendus Physique, 2009, 10, 469-490.	0.9	22
293	Fingerprints of Bonding Motifs in DNA Duplexes of Adenine and Thymine Revealed from Circular Dichroism: Synchrotron Radiation Experiments and TDDFT Calculations. Journal of Physical Chemistry B, 2009, 113, 9614-9619.	2.6	17
294	Modified Ehrenfest Formalism for Efficient Large-Scale ab initio Molecular Dynamics. Journal of Chemical Theory and Computation, 2009, 5, 728-742.	5.3	124
295	Optical and Vibrational Properties of Boron Nitride Nanotubes. , 2009, , 105-148.		12
296	Towards a gauge invariant method for molecular chiroptical properties in TDDFT. Physical Chemistry Chemical Physics, 2009, 11, 4481.	2.8	46
297	Hot-electron-assisted femtochemistry at surfaces: A time-dependent density functional theory approach. Physical Review B, 2009, 79, .	3.2	18
298	Ab initio electronic and optical spectra of free-base porphyrins: The role of electronic correlation. Journal of Chemical Physics, 2009, 131, 084102.	3.0	120
299	Conserving<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:mi>G</mml:mi><mml:mi>W</mml:mi></mml:mrow></mml:math>scheme for nonequilibrium quantum transport in molecular contacts. Physical Review B, 2008, 77, .	3.2	204
300	Conductance of Sidewall-Functionalized Carbon Nanotubes: Universal Dependence on Adsorption Sites. Physical Review Letters, 2008, 101, 236806.	7.8	41
301	Ab initiostudy of transport properties in defected carbon nanotubes: an O(N) approach. Journal of Physics Condensed Matter, 2008, 20, 294214.	1.8	22
302	Optical Saturation Driven by Exciton Confinement in Molecular Chains: A Time-Dependent Density-Functional Theory Approach. Physical Review Letters, 2008, 101, 133002.	7.8	47
303	Ab initiostudy of the dielectric response of crystalline ropes of metallic single-walled carbon nanotubes: Tube-diameter and helicity effects. Physical Review B, 2008, 78, .	3.2	16
304	The role of dimensionality on the quenching of spin-orbit effects in the optics of gold nanostructures. Journal of Chemical Physics, 2008, 129, 144110.	3.0	36
305	Comment on â€œHuge Excitonic Effects in Layered Hexagonal Boron Nitrideâ€• Physical Review Letters, 2008, 100, 189701; discussion 189702.	7.8	64
306	Ultrafast electron-phonon decoupling in graphite. Physical Review B, 2008, 77, .	3.2	120

#	Article	IF	Citations
307	Cluster-surface and cluster-cluster interactions:Ab initiocalculations and modeling of asymptotic van der Waals forces. Physical Review B, 2008, 78, .	3.2	26
308	Time-dependent density functional theory scheme for efficient calculations of dynamic (hyper)polarizabilities. Journal of Chemical Physics, 2007, 126, 184106.	3.0	106
309	Microscopic investigation of laser-induced structural changes in single-wall carbon nanotubes. Physical Review B, 2007, 75, .	3.2	15
310	Identification of a gene-pathway associated with non-alcoholic steatohepatitis. Journal of Hepatology, 2007, 46, 708-718.	3.7	52
311	Nonequilibrium GW approach to quantum transport in nano-scale contacts. Journal of Chemical Physics, 2007, 126, 091101.	3.0	100
312	Advanced Correlation Functionals:â€‰ Application to Bulk Materials and Localized Systems. Journal of Physical Chemistry A, 2007, 111, 12458-12465.	2.5	35
313	Absorption of BN nanotubes under the influence of a perpendicular electric field. Physica Status Solidi (B): Basic Research, 2007, 244, 4288-4292.	1.5	22
314	Excitons in Boron Nitride Nanotubes: Dimensionality Effects. Physical Review Letters, 2006, 96, 126104.	7.8	343
315	Real-TimeAbÂInitioSimulations of Excited Carrier Dynamics in Carbon Nanotubes. Physical Review Letters, 2006, 97, 126104.	7.8	47
316	Asymptotics of the Dispersion Interaction: Analytic Benchmarks for van der Waals Energy Functionals. Physical Review Letters, 2006, 96, 073201.	7.8	314
317	A TDDFT Study of the Excited States of DNA Bases and Their Assemblies. Journal of Physical Chemistry B, 2006, 110, 7129-7138.	2.6	112
318	Density functionals from many-body perturbation theory: The band gap for semiconductors and insulators. Journal of Chemical Physics, 2006, 124, 154108.	3.0	166
319	Electronic structure and excitations in oligoacenes from ab initio calculations. Journal of Chemical Physics, 2006, 124, 134901.	3.0	103
320	Exact Coulomb cutoff technique for supercell calculations. Physical Review B, 2006, 73, .	3.2	369
321	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
322	Electronic Structure Calculations for Nanomolecular Systems. , 2006, , 77-116.		3
323	First-Principles Description of Correlation Effects in Layered Materials. Physical Review Letters, 2006, 96, 136404.	7.8	183
324	Effect of spatial nonlocality on the density functional band gap. Physical Review B, 2006, 74, .	3.2	68

#	Article	IF	Citations
325	TDDFT from molecules to solids: The role of long-range interactions. International Journal of Quantum Chemistry, 2005, 102, 684-701.	2.0	65
326	Raman spectra of BN nanotubes:Ab initioand bond-polarizability model calculations. Physical Review B, 2005, 71, .	3.2	40
327	Anderson Localization in Carbon Nanotubes: Defect Density and Temperature Effects. Physical Review Letters, 2005, 95, 266801.	7.8	65
328	Optical Absorption of the Blue Fluorescent Protein: A First-Principles Study. Journal of the American Chemical Society, 2005, 127, 12329-12337.	13.7	69
329	Quasiparticle and Optical Properties of Solids and Nanostructures: The GW-BSE Approach. , 2005, , 215-240.		15
330	Photodesorption of oxygen from carbon nanotubes. Physical Review B, 2004, 70, .	3.2	19
331	Electron linewidths of wide-gap insulators: Excitonic effects inLiF. Physical Review B, 2004, 70, .	3.2	16
332	Ab initiostudy of the optical absorption and wave-vector-dependent dielectric response of graphite. Physical Review B, 2004, 69, .	3.2	175
333	The phonon dispersion of graphite revisited. Solid State Communications, 2004, 131, 141-152.	1.9	314
334	Can photo excitations heal defects in carbon nanotubes?. Chemical Physics Letters, 2004, 392, 209-213.	2.6	23
335	Long-range contribution to the exchange-correlation kernel of time-dependent density functional theory. Physical Review B, 2004, 69, .	3.2	184
336	Electrical transport in carbon nanotubes: Role of disorder and helical symmetries. Physical Review B, 2004, 69, .	3.2	149
337	Propagators for the time-dependent Kohnâ€“Sham equations. Journal of Chemical Physics, 2004, 121, 3425-3433.	3.0	477
338	Spectroscopic characterization of Stone-Wales defects in nanotubes. Physical Review B, 2004, 69, .	3.2	134
339	Time and energy-resolved two photon photoemission of the Cu(100) and Cu(111) metal surfaces. Computational Materials Science, 2004, 30, 110-115.	3.0	11
340	Optical Properties of Nanostructures from Time-Dependent Density Functional Theory. Journal of Computational and Theoretical Nanoscience, 2004, 1, 231-255.	0.4	21
341	Application of the Electronic Properties of Carbon Nanotubes: Computation of the Magnetic Properties and the 13C NMR Shifts. , 2004, , 343-358.		0
342	octopus: a first-principles tool for excited electronâ€“ion dynamics. Computer Physics Communications, 2003, 151, 60-78.	7.5	671

#	Article	IF	Citations
343	Ab initiocalculations of the lattice dynamics of boron nitride nanotubes. Physical Review B, 2003, 68, .	3.2	165
344	Time-Dependent Density-Functional Approach for Biological Chromophores: The Case of the Green Fluorescent Protein. Physical Review Letters, 2003, 90, 258101.	7.8	181
345	Optical and Loss Spectra of Carbon Nanotubes: Depolarization Effects and Intertube Interactions. Physical Review Letters, 2003, 91, 046402.	7.8	174
346	High-pressure phases of group-IV, IIIâ€“V, and IIâ€“VI compounds. Reviews of Modern Physics, 2003, 75, 863-912.	45.6	922
347	Band structure of boron doped carbon nanotubes. AIP Conference Proceedings, 2003, , .	0.4	23
348	Functional proteomics of nonalcoholic steatohepatitis: Mitochondrial proteins as targets of S -adenosylmethionine. Proceedings of the National Academy of Sciences of the United States of America, 2003, 100, 3065-3070.	7.1	154
349	Persistent currents in carbon nanotube based rings. Physical Review B, 2003, 67, .	3.2	72
350	Bound Excitons in Time-Dependent Density-Functional Theory: Optical and Energy-Loss Spectra. Physical Review Letters, 2003, 91, 256402.	7.8	151
351	GARBAN: genomic analysis and rapid biological annotation of cDNA microarray and proteomic data. Bioinformatics, 2003, 19, 2158-2160.	4.1	27
352	Patching and Tearing Single-Wall Carbon-Nanotube Ropes into Multiwall Carbon Nanotubes. Physical Review Letters, 2002, 89, 255501.	7.8	52
353	Can optical spectroscopy directly elucidate the ground state of C20?. Journal of Chemical Physics, 2002, 116, 1930-1933.	3.0	55
354	Quasiparticle band-structure effects on thedhole lifetimes of copper within theGWapproximation. Physical Review B, 2002, 66, .	3.2	32
355	Electronic excitations: density-functional versus many-body Greenâ€™s-function approaches. Reviews of Modern Physics, 2002, 74, 601-659.	45.6	3,375
356	Excitonic Effects in Solids Described by Time-Dependent Density-Functional Theory. Physical Review Letters, 2002, 88, 066404.	7.8	282
357	Onset of nanotube decay under extreme thermal and electronic excitations. Physica B: Condensed Matter, 2002, 323, 78-85.	2.7	37
358	Mechanical properties of carbon nanotubes: a fiber digest for beginners. Carbon, 2002, 40, 1729-1734.	10.3	373
359	Anisotropy and Interplane Interactions in the Dielectric Response of Graphite. Physical Review Letters, 2002, 89, 076402.	7.8	119
360	Prediction of Dispersion Forces: Is There a Problem?. Australian Journal of Chemistry, 2001, 54, 513.	0.9	148

#	Article	IF	Citations
361	Electronic conduction in multi-walled carbon nanotubes: role of intershell coupling and incommensurability. Physics Letters, Section A: General, Atomic and Solid State Physics, 2001, 285, 94-100.	2.1	48
362	C13NMR Chemical Shift of Single-Wall Carbon Nanotubes. Physical Review Letters, 2001, 86, 3160-3163.	7.8	58
363	Stochastic Heterostructures and Diodium in B/N-Doped Carbon Nanotubes. Physical Review Letters, 2001, 87, 136402.	7.8	59
364	Influence of packing on the vibrational properties of infinite and finite bundles of carbon nanotubes. Physical Review B, 2001, 64, .	3.2	33
365	Conduction mechanisms and magnetotransport in multiwalled carbon nanotubes. Physical Review B, 2001, 64, .	3.2	111
366	Assessment of exchange-correlation functionals for the calculation of dynamical properties of small clusters in time-dependent density functional theory. Journal of Chemical Physics, 2001, 115, 3006-3014.	3.0	172
367	Anomalous Quasiparticle Lifetime in Graphite: Band Structure Effects. Physical Review Letters, 2001, 87, 246405.	7.8	62
368	Boron Quasicrystals and Boron Nanotubes: Ab Initio Study of Various B96 Isomers. Journal of Solid State Chemistry, 2000, 154, 269-274.	2.9	51
369	Mechanical and electronic properties of carbon and boronâ€“nitride nanotubes. Carbon, 2000, 38, 1681-1690.	10.3	171
370	Real-space, real-time method for the dielectric function. Physical Review B, 2000, 62, 7998-8002.	3.2	326
371	Theoretical study of the relative stability of structural phases in group-III nitrides at high pressures. Physical Review B, 2000, 62, 16612-16623.	3.2	196
372	Lowest excitation energy in atoms in the adiabatic approximation related to the single-particle kinetic energy functional. Journal of Physics B: Atomic, Molecular and Optical Physics, 1999, 32, 2173-2179.	1.5	9
373	Self-inductance of chiral conducting nanotubes. Physical Review B, 1999, 60, 13885-13889.	3.2	26
374	New boron based nanostructured materials. Journal of Chemical Physics, 1999, 110, 3176-3185.	3.0	257
375	Ab initio study of B32 clusters: competition between spherical, quasiplanar and tubular isomers. Chemical Physics Letters, 1999, 311, 21-28.	2.6	105
376	Ab initiostructural, elastic, and vibrational properties of carbon nanotubes. Physical Review B, 1999, 59, 12678-12688.	3.2	854
377	Electronic States in a Finite Carbon Nanotube: A One-Dimensional Quantum Box. Physical Review Letters, 1999, 82, 3520-3523.	7.8	173
378	van der Waals interaction in nanotube bundles: Consequences on vibrational modes. Physical Review B, 1999, 60, R8521-R8524.	3.2	206

#	Article	IF	Citations
379	Generalized time-dependent density-functional theory including core polarization. European Physical Journal D, 1998, 48, 756-759.	0.4	0
380	SMALL BAND-GAP GRAPHITIC CBN LAYERS. Journal of Physics and Chemistry of Solids, 1998, 59, 1303-1308.	4.0	22
381	Reversible bending of carbon nanotubes using a transmission electron microscope. Applied Physics Letters, 1998, 73, 1961-1963.	3.3	41
382	Core Polarization in the Optical Response of Metal Clusters: Generalized Time-Dependent Density-Functional Theory. Physical Review Letters, 1997, 78, 1428-1431.	7.8	54
383	Theoretical Models for the Optical Properties of Clusters and Nanostructures. International Journal of Modern Physics B, 1997, 11, 2727-2776.	2.0	25
384	In SituBand Gap Engineering of Carbon Nanotubes. Physical Review Letters, 1997, 79, 2093-2096.	7.8	273
385	Ab initio calculations of the pressure-induced structural phase transitionsfor four II-VI compounds. Physical Review B, 1997, 55, 13025-13031.	3.2	191
386	Electronic and Doping Properties of B x C y N z Nanotubes. , 1997, , 133-142.		1
387	Optical response of Ag clusters. , 1997, , 262-264.		0
388	Theoretical study of one-dimensional chains of metal atoms in nanotubes. Physical Review B, 1996, 53, 4023-4026.	3.2	93
389	Ab InitioPhotoabsorption Spectra and Structures of Small Semiconductor and Metal Clusters. Physical Review Letters, 1996, 77, 247-250.	7.8	193
390	Density-functional theory of the nonlinear optical susceptibility: Application to cubic semiconductors. Physical Review B, 1996, 53, 15638-15642.	3.2	103
391	Calculated structural and electronic properties of CdSe under pressure. Physical Review B, 1995, 51, 4926-4930.	3.2	50
392	Mixed-space formalism for the dielectric response in periodic systems. Physical Review B, 1995, 52, R2225-R2228.	3.2	37
393	Synthesis ofBxCyNznanotubules. Physical Review B, 1995, 51, 11229-11232.	3.2	413
394	Quasiparticle excitations inGaAs1â^'xNxandAlAs1â^'xNxordered alloys. Physical Review B, 1995, 51, 4343-4346.	3.2	96
395	Quasiparticle band structure of bulk hexagonal boron nitride and related systems. Physical Review B, 1995, 51, 6868-6875.	3.2	583
396	Ionic Cohesion and Electron Doping of Thin Carbon Tubules with Alkali Atoms. Physical Review Letters, 1995, 74, 2993-2996.	7.8	163

#	Article	IF	Citations
397	Quasiparticle band structures of short-period superlattices and ordered alloys of AlN and GaN. Physical Review B, 1994, 49, 1952-1956.	3.2	44
398	Theory of graphitic boron nitride nanotubes. Physical Review B, 1994, 49, 5081-5084.	3.2	1,564
399	Quasiparticle band structures of six II-VI compounds: ZnS, ZnSe, ZnTe, CdS, CdSe, and CdTe. Physical Review B, 1994, 50, 10780-10787.	3.2	366
400	Chiral tubules of hexagonalBC2N. Physical Review B, 1994, 50, 4976-4979.	3.2	343
401	Electronic properties of tubule forms of hexagonalBC3. Physical Review B, 1994, 50, 18360-18366.	3.2	236
402	Collective excitations of embedded potassium clusters. Zeitschrift FÃ¼r Physik D-Atoms Molecules and Clusters, 1993, 26, 122-124.	1.0	7
403	Quasiparticle band structure of AlN and GaN. Physical Review B, 1993, 48, 11810-11816.	3.2	328
404	Dielectric screening effects on the photoabsorption cross section of embedded metallic clusters. Physical Review B, 1993, 48, 18222-18229.	3.2	48
405	Ultrafast dynamics of adenine following XUV ionization. JPhys Photonics, 0, , .	4.6	2
406	Ab Initio Cluster Approach for High Harmonic Generation in Liquids. Journal of Chemical Theory and Computation, 0, , .	5.3	14
407	Entangled Biphoton Enhanced Double Quantum Coherence Signal as a Probe for Cavity Polariton Correlations in Presence of Phonon Induced Dephasing. Frontiers in Physics, 0, 10, .	2.1	1