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	Electronic excitations: density-functional versus many-body Greenâ€™s-function approaches. Reviews of Modern Physics, 2002, 74, 601-659.	45.6	3,375
2	Theory of graphitic boron nitride nanotubes. Physical Review B, 1994, 49, 5081-5084.	3.2	1,564
3	High-pressure phases of group-IV, IIIâ€“V, and IIâ€“VI compounds. Reviews of Modern Physics, 2003, 75, 863-912.	45.6	922
4	Ab initiostructural, elastic, and vibrational properties of carbon nanotubes. Physical Review B, 1999, 59, 12678-12688.	3.2	854
5	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
6	octopus: a first-principles tool for excited electronâ€“ion dynamics. Computer Physics Communications, 2003, 151, 60-78.	7.5	671
7	Maximized electron interactions at the magic angle in twisted bilayer graphene. Nature, 2019, 572, 95-100.	27.8	644
8	Quasiparticle band structure of bulk hexagonal boron nitride and related systems. Physical Review B, 1995, 51, 6868-6875.	3.2	583
9	Correlated electronic phases in twisted bilayer transition metal dichalcogenides. Nature Materials, 2020, 19, 861-866.	27.5	544
10	Direct Imaging of Covalent Bond Structure in Single-Molecule Chemical Reactions. Science, 2013, 340, 1434-1437.	12.6	513
11	Propagators for the time-dependent Kohnâ€“Sham equations. Journal of Chemical Physics, 2004, 121, 3425-3433.	3.0	477
12	Dielectric screening in two-dimensional insulators: Implications for excitonic and impurity states in graphane. Physical Review B, 2011, 84, .	3.2	476
13	Coherent ultrafast charge transfer in an organic photovoltaic blend. Science, 2014, 344, 1001-1005.	12.6	470
14	Synthesis ofBxCyNznanotubules. Physical Review B, 1995, 51, 11229-11232.	3.2	413
15	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
16	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
17	Mechanical properties of carbon nanotubes: a fiber digest for beginners. Carbon, 2002, 40, 1729-1734.	10.3	373
18	Exact Coulomb cutoff technique for supercell calculations. Physical Review B, 2006, 73, .	3.2	369

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19	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
20	Chiral tubules of hexagonalBC2N. Physical Review B, 1994, 50, 4976-4979.	3.2	343
21	Excitons in Boron Nitride Nanotubes: Dimensionality Effects. Physical Review Letters, 2006, 96, 126104.	7.8	343
22	Confined linear carbon chains as a route to bulkÂcarbyne. Nature Materials, 2016, 15, 634-639.	27.5	341
23	Quasiparticle band structure of AlN and GaN. Physical Review B, 1993, 48, 11810-11816.	3.2	328
24	Real-space, real-time method for the dielectric function. Physical Review B, 2000, 62, 7998-8002.	3.2	326
25	MoirÃ© heterostructures as a condensed-matter quantum simulator. Nature Physics, 2021, 17, 155-163.	16.7	317
26	The phonon dispersion of graphite revisited. Solid State Communications, 2004, 131, 141-152.	1.9	314
27	Asymptotics of the Dispersion Interaction: Analytic Benchmarks for van der Waals Energy Functionals. Physical Review Letters, 2006, 96, 073201.	7.8	314
28	Excitonic Effects in Solids Described by Time-Dependent Density-Functional Theory. Physical Review Letters, 2002, 88, 066404.	7.8	282
29	In SituBand Gap Engineering of Carbon Nanotubes. Physical Review Letters, 1997, 79, 2093-2096.	7.8	273
30	New boron based nanostructured materials. Journal of Chemical Physics, 1999, 110, 3176-3185.	3.0	257
31	Creating stable Floquetâ€“Weyl semimetals by laser-driving of 3D Dirac materials. Nature Communications, 2017, 8, 13940.	12.8	255
32	The physical and chemical properties of heteronanotubes. Reviews of Modern Physics, 2010, 82, 1843-1885.	45.6	239
33	Quantum coherence controls the charge separation in a prototypical artificial light-harvesting system. Nature Communications, 2013, 4, 1602.	12.8	239
34	Electronic properties of tubule forms of hexagonalBC3. Physical Review B, 1994, 50, 18360-18366.	3.2	236
35	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
36	Impact of the Electronic Band Structure in High-Harmonic Generation Spectra of Solids. Physical Review Letters, 2017, 118, 087403.	7.8	226

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37	Artificially Stacked Atomic Layers: Toward New van der Waals Solids. Nano Letters, 2012, 12, 3518-3525.	9.1	211
38	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
39	van der Waals interaction in nanotube bundles: Consequences on vibrational modes. Physical Review B, 1999, 60, R8521-R8524.	3.2	206
40	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
41	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></mml:mrow> to Photocarrier Doping. Physical Review Letters, 2014, 113, 216401.	7.8	203
42	Quantum-electrodynamical density-functional theory: Bridging quantum optics and electronic-structure theory. Physical Review A, 2014, 90, .	2.5	197
43	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
44	Ab InitioPhotoabsorption Spectra and Structures of Small Semiconductor and Metal Clusters. Physical Review Letters, 1996, 77, 247-250.	7.8	193
45	Ab initio calculations of the pressure-induced structural phase transitionsfor four II-VI compounds. Physical Review B, 1997, 55, 13025-13031.	3.2	191
46	Long-range contribution to the exchange-correlation kernel of time-dependent density functional theory. Physical Review B, 2004, 69, .	3.2	184
47	Computing the shortest elementary flux modes in genome-scale metabolic networks. Bioinformatics, 2009, 25, 3158-3165.	4.1	184
48	First-Principles Description of Correlation Effects in Layered Materials. Physical Review Letters, 2006, 96, 136404.	7.8	183
49	From a quantum-electrodynamical lightâ€“matter description to novel spectroscopies. Nature Reviews Chemistry, 2018, 2, .	30.2	182
50	Time-Dependent Density-Functional Approach for Biological Chromophores: The Case of the Green Fluorescent Protein. Physical Review Letters, 2003, 90, 258101.	7.8	181
51	Time-dependent density-functional theory in massively parallel computer architectures: the octopus project. Journal of Physics Condensed Matter, 2012, 24, 233202.	1.8	181
52	Strong Charge-Transfer Excitonic Effects and the Bose-Einstein Exciton Condensate in Graphane. Physical Review Letters, 2010, 104, 226804.	7.8	180
53	Ab initiostudy of the optical absorption and wave-vector-dependent dielectric response of graphite. Physical Review B, 2004, 69, .	3.2	175
54	Optical and Loss Spectra of Carbon Nanotubes: Depolarization Effects and Intertube Interactions. Physical Review Letters, 2003, 91, 046402.	7.8	174

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55	Electronic States in a Finite Carbon Nanotube: A One-Dimensional Quantum Box. Physical Review Letters, 1999, 82, 3520-3523.	7.8	173
56	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
57	Mechanical and electronic properties of carbon and boronâ€“nitride nanotubes. Carbon, 2000, 38, 1681-1690.	10.3	171
58	Density functionals from many-body perturbation theory: The band gap for semiconductors and insulators. Journal of Chemical Physics, 2006, 124, 154108.	3.0	166
59	Ab initiocalculations of the lattice dynamics of boron nitride nanotubes. Physical Review B, 2003, 68, .	3.2	165
60	Ionic Cohesion and Electron Doping of Thin Carbon Tubules with Alkali Atoms. Physical Review Letters, 1995, 74, 2993-2996.	7.8	163
61	Polariton panorama. Nanophotonics, 2020, 10, 549-577.	6.0	155
62	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
63	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
64	Bound Excitons in Time-Dependent Density-Functional Theory: Optical and Energy-Loss Spectra. Physical Review Letters, 2003, 91, 256402.	7.8	151
65	Electrical transport in carbon nanotubes: Role of disorder and helical symmetries. Physical Review B, 2004, 69, .	3.2	149
66	Prediction of Dispersion Forces: Is There a Problem?. Australian Journal of Chemistry, 2001, 54, 513.	0.9	148
67	Ab initionanoplasmonics: The impact of atomic structure. Physical Review B, 2014, 90, .	3.2	147
68	Ellipticity dependence of high-harmonic generation in solids originating from coupled intraband and interband dynamics. Nature Communications, 2017, 8, 745.	12.8	146
69	Enhanced thermoelectric properties in hybrid graphene/boron nitride nanoribbons. Physical Review B, 2012, 86, .	3.2	138
70	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
71	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
72	Spectroscopic characterization of Stone-Wales defects in nanotubes. Physical Review B, 2004, 69, .	3.2	134

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73	Cavity Bornâ€“Oppenheimer Approximation for Correlated Electronâ€“Nuclear-Photon Systems. Journal of Chemical Theory and Computation, 2017, 13, 1616-1625.	5.3	133
74	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
75	Imaging single-molecule reaction intermediates stabilized by surface dissipation and entropy. Nature Chemistry, 2016, 8, 678-683.	13.6	130
76	Ab initiononrelativistic quantum electrodynamics: Bridging quantum chemistry and quantum optics from weak to strong coupling. Physical Review A, 2018, 98, .	2.5	126
77	Modified Ehrenfest Formalism for Efficient Large-Scale ab initio Molecular Dynamics. Journal of Chemical Theory and Computation, 2009, 5, 728-742.	5.3	124
78	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
79	Ultrafast electron-phonon decoupling in graphite. Physical Review B, 2008, 77, .	3.2	120
80	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
81	Engineering quantum materials with chiral optical cavities. Nature Materials, 2021, 20, 438-442.	27.5	120
82	Anisotropy and Interplane Interactions in the Dielectric Response of Graphite. Physical Review Letters, 2002, 89, 076402.	7.8	119
83	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
84	Quantum plasmonics: from jellium models to ab initio calculations. Nanophotonics, 2016, 5, 409-426.	6.0	116
85	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
86	Conduction mechanisms and magnetotransport in multiwalled carbon nanotubes. Physical Review B, 2001, 64, .	3.2	111
87	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
88	Time-dependent density functional theory scheme for efficient calculations of dynamic (hyper)polarizabilities. Journal of Chemical Physics, 2007, 126, 184106.	3.0	106
89	Ab initio study of B32 clusters: competition between spherical, quasiplanar and tubular isomers. Chemical Physics Letters, 1999, 311, 21-28.	2.6	105
90	Relevance of the Quadratic Diamagnetic and Self-Polarization Terms in Cavity Quantum Electrodynamics. ACS Photonics, 2020, 7, 975-990.	6.6	105

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91	Density-functional theory of the nonlinear optical susceptibility: Application to cubic semiconductors. Physical Review B, 1996, 53, 15638-15642.	3.2	103
92	Electronic structure and excitations in oligoacenes from ab initio calculations. Journal of Chemical Physics, 2006, 124, 134901.	3.0	103
93	Performance of Nonlocal Optics When Applied to Plasmonic Nanostructures. Journal of Physical Chemistry C, 2013, 117, 8941-8949.	3.1	103
94	Coupled Cluster Theory for Molecular Polaritons: Changing Ground and Excited States. Physical Review X, 2020, 10, .	8.9	102
95	Nonequilibrium GW approach to quantum transport in nano-scale contacts. Journal of Chemical Physics, 2007, 126, 091101.	3.0	100
96	Excitons in molecular crystals from first-principles many-body perturbation theory: Picene versus pentacene. Physical Review B, 2012, 86, .	3.2	99
97	Atomic-like high-harmonic generation from two-dimensional materials. Science Advances, 2018, 4, eaao5207.	10.3	98
98	Quasiparticle excitations inGaAs1â^'xNxandAlAs1â^'xNxordered alloys. Physical Review B, 1995, 51, 4343-4346.	3.2	96
99	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
100	Theoretical study of one-dimensional chains of metal atoms in nanotubes. Physical Review B, 1996, 53, 4023-4026.	3.2	93
101	Optimized Effective Potential for Quantum Electrodynamical Time-Dependent Density Functional Theory. Physical Review Letters, 2015, 115, 093001.	7.8	93
102	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
103	Phonon-driven spin-Floquet magneto-valleytronics in MoS2. Nature Communications, 2018, 9, 638.	12.8	86
104	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
105	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
106	Intermolecular interactions in optical cavities: An ab initio QED study. Journal of Chemical Physics, 2021, 154, 094113.	3.0	81
107	Lightâ€“Matter Response in Nonrelativistic Quantum Electrodynamics. ACS Photonics, 2019, 6, 2757-2778.	6.6	79
108	Understanding Energy-Level Alignment in Donorâ€“Acceptor/Metal Interfaces from Core-Level Shifts. ACS Nano, 2013, 7, 6914-6920.	14.6	78

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109	Identification of Alternative Splicing Events Regulated by the Oncogenic Factor SRSF1 in Lung Cancer. Cancer Research, 2014, 74, 1105-1115.	0.9	77
110	Exciton dispersion in molecular solids. Journal of Physics Condensed Matter, 2015, 27, 113204.	1.8	74
111	Emergent elemental two-dimensional materials beyond graphene. Journal Physics D: Applied Physics, 2017, 50, 053004.	2.8	74
112	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> Physical Review Letters, 2020, 124, 197601.	7.8	73
113	Enhanced tunable second harmonic generation from twistable interfaces and vertical superlattices in boron nitride homostructures. Science Advances, 2021, 7, .	10.3	73
114	Persistent currents in carbon nanotube based rings. Physical Review B, 2003, 67, .	3.2	72
115	Optical Absorption of the Blue Fluorescent Protein: A First-Principles Study. Journal of the American Chemical Society, 2005, 127, 12329-12337.	13.7	69
116	Mechanically Interlocked Singleâ€Wall Carbon Nanotubes. Angewandte Chemie - International Edition, 2014, 53, 5394-5400.	13.8	69
117	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
118	Effect of spatial nonlocality on the density functional band gap. Physical Review B, 2006, 74, .	3.2	68
119	Level Alignment of a Prototypical Photocatalytic System: Methanol on TiO₂(110). Journal of the American Chemical Society, 2013, 135, 11429-11432.	13.7	68
120	Many-Body Effects in the Excitation Spectrum of a Defect in SiC. Physical Review Letters, 2010, 105, 026401.	7.8	66
121	Strongly correlated electronâ€“photon systems. Nature, 2022, 606, 41-48.	27.8	66
122	TDDFT from molecules to solids: The role of long-range interactions. International Journal of Quantum Chemistry, 2005, 102, 684-701.	2.0	65
123	Anderson Localization in Carbon Nanotubes: Defect Density and Temperature Effects. Physical Review Letters, 2005, 95, 266801.	7.8	65
124	Nanoscale patchworks. Nature Materials, 2010, 9, 379-380.	27.5	65
125	Role of nonlocal exchange in the electronic structure of correlated oxides. Physical Review B, 2012, 85, .	3.2	65
126	Cavity Control of Excitons in Two-Dimensional Materials. Nano Letters, 2019, 19, 3473-3479.	9.1	65

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127	Polaritonic Chemistry: Collective Strong Coupling Implies Strong Local Modification of Chemical Properties. Journal of Physical Chemistry Letters, 2021, 12, 508-516.	4.6	65
128	Comment on â€œHuge Excitonic Effects in Layered Hexagonal Boron Nitrideâ€• Physical Review Letters, 2008, 100, 189701; discussion 189702.	7.8	64
129	Structure, electronic, and optical properties of TiO2 atomic clusters: An ab initio study. Journal of Chemical Physics, 2011, 135, 244704.	3.0	64
130	Modeling electron dynamics coupled to continuum states in finite volumes with absorbing boundaries. European Physical Journal B, 2015, 88, 1.	1.5	64
131	Monitoring Electron-Photon Dressing in WSe₂. Nano Letters, 2016, 16, 7993-7998.	9.1	64
132	Phonon Driven Floquet Matter. Nano Letters, 2018, 18, 1535-1542.	9.1	63
133	Anomalous Quasiparticle Lifetime in Graphite: Band Structure Effects. Physical Review Letters, 2001, 87, 246405.	7.8	62
134	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
135	Sodium: A Charge-Transfer Insulator at High Pressures. Physical Review Letters, 2010, 104, 216404.	7.8	61
136	Electronic band gaps of confined linear carbon chains ranging from polyyne to carbyne. Physical Review Materials, 2017, 1, .	2.4	61
137	Quasiparticle Level Alignment for Photocatalytic Interfaces. Journal of Chemical Theory and Computation, 2014, 10, 2103-2113.	5.3	60
138	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
139	MoirÃ© metrology of energy landscapes in van der Waals heterostructures. Nature Communications, 2021, 12, 242.	12.8	60
140	Stochastic Heterostructures and Diodium in B/N-Doped Carbon Nanotubes. Physical Review Letters, 2001, 87, 136402.	7.8	59
141	Silicite: The layered allotrope of silicon. Physical Review B, 2014, 90, .	3.2	59
142	MoirÃ©less correlations in ABCA graphene. Proceedings of the National Academy of Sciences of the United States of America, 2021, 118, .	7.1	59
143	C13NMR Chemical Shift of Single-Wall Carbon Nanotubes. Physical Review Letters, 2001, 86, 3160-3163.	7.8	58
144	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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145	Polaritonic coupled-cluster theory. Physical Review Research, 2020, 2, .	3.6	57
146	Realization of nearly dispersionless bands with strong orbital anisotropy from destructive interference in twisted bilayer MoS2. Nature Communications, 2021, 12, 5644.	12.8	57
147	Higher-Order Band Topology in Twisted MoirÃ© Superlattice. Physical Review Letters, 2021, 126, 066401.	7.8	56
148	Topological Floquet engineering of twisted bilayer graphene. Physical Review Research, 2019, 1, .	3.6	56
149	Can optical spectroscopy directly elucidate the ground state of C20?. Journal of Chemical Physics, 2002, 116, 1930-1933.	3.0	55
150	Unraveling the Intrinsic Color of Chlorophyll. Angewandte Chemie - International Edition, 2015, 54, 2170-2173.	13.8	55
151	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
152	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></mml:m Physical Review B, 2015, 91, .	3.2	54
153	High-harmonic generation from few-layer hexagonal boron nitride: Evolution from monolayer to bulk response. Physical Review B, 2018, 98, .	3.2	54
154	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
155	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
156	Charge-Transfer Plasmon Polaritons at Graphene/Î±-RuCl₃ Interfaces. Nano Letters, 2020, 20, 8438-8445.	9.1	53
157	Universal slow plasmons and giant field enhancement in atomically thin quasi-two-dimensional metals. Nature Communications, 2020, 11, 1013.	12.8	53
158	Patching and Tearing Single-Wall Carbon-Nanotube Ropes into Multiwall Carbon Nanotubes. Physical Review Letters, 2002, 89, 255501.	7.8	52
159	Identification of a gene-pathway associated with non-alcoholic steatohepatitis. Journal of Hepatology, 2007, 46, 708-718.	3.7	52
160	Customized Electronic Coupling in Selfâ€Assembled Donorâ€“Acceptor Nanostructures. Advanced Functional Materials, 2009, 19, 3567-3573.	14.9	52
161	Boron Quasicrystals and Boron Nanotubes: Ab Initio Study of Various B96 Isomers. Journal of Solid State Chemistry, 2000, 154, 269-274.	2.9	51
162	MoirÃ© nematic phase in twisted double bilayer graphene. Nature Physics, 2022, 18, 196-202.	16.7	51

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163	Calculated structural and electronic properties of CdSe under pressure. Physical Review B, 1995, 51, 4926-4930.	3.2	50
164	Comparing Quasiparticle H₂O Level Alignment on Anatase and Rutile TiO₂. ACS Catalysis, 2015, 5, 4242-4254.	11.2	50
165	Frenkel versus charge-transfer exciton dispersion in molecular crystals. Physical Review B, 2013, 88, .	3.2	49
166	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
167	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
168	Dielectric screening effects on the photoabsorption cross section of embedded metallic clusters. Physical Review B, 1993, 48, 18222-18229.	3.2	48
169	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
170	High-harmonic generation from spin-polarised defects in solids. Npj Computational Materials, 2020, 6, .	8.7	48
171	Real-TimeAbÂInitioSimulations of Excited Carrier Dynamics in Carbon Nanotubes. Physical Review Letters, 2006, 97, 126104.	7.8	47
172	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
173	Towards a gauge invariant method for molecular chiroptical properties in TDDFT. Physical Chemistry Chemical Physics, 2009, 11, 4481.	2.8	46
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