

# Angel Rubio

## List of Publications by Year in descending order

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407  
papers

37,234  
citations

2669

95  
h-index

3638

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. <i>Physical Review Research</i> , 2022, 4, .	1.3	33
2	Detecting multiple chiral centers in chiral molecules with high harmonic generation. <i>Optics Express</i> , 2022, 30, 3729.	1.7	16
3	Moiré engineering of spin-orbit coupling in twisted platinum diselenide. <i>Electronic Structure</i> , 2022, 4, 014004.	1.0	8
4	First-principles modelling for time-resolved ARPES under different pump-probe conditions. <i>Journal of Electron Spectroscopy and Related Phenomena</i> , 2022, 254, 147152.	0.8	9
5	Nanometer-Scale Lateral p-n Junctions in Graphene/RuCl <sub>3</sub> Heterostructures. <i>Nano Letters</i> , 2022, 22, 1946-1953.	4.5	25
6	Cavity-Modulated Proton Transfer Reactions. <i>Journal of the American Chemical Society</i> , 2022, 144, 4995-5002.	6.6	32
7	TMDs as a platform for spin liquid physics: A strong coupling study of twisted bilayer WSe <sub>2</sub> . <i>APL Materials</i> , 2022, 10, .	2.2	19
8	A new Hall for quantum protection. <i>Science</i> , 2022, 375, 976-977.	6.0	4
9	Microscopic theory of light-induced ultrafast skyrmion excitation in transition metal films. <i>Npj Computational Materials</i> , 2022, 8, .	3.5	8
10	Comment on "Origin of symmetry-forbidden high-order harmonic generation in the time-dependent Kohn-Sham formulation". <i>Physical Review A</i> , 2022, 105, .	1.0	1
11	Moiré nematic phase in twisted double bilayer graphene. <i>Nature Physics</i> , 2022, 18, 196-202.	6.5	51
12	Polaritonic Hofstadter butterfly and cavity control of the quantized Hall conductance. <i>Physical Review B</i> , 2022, 105, .	1.1	20
13	A perspective on <i>ab initio</i> modeling of polaritonic chemistry: The role of non-equilibrium effects and quantum collectivity. <i>Journal of Chemical Physics</i> , 2022, 156, .	1.2	39
14	Strongly correlated electron-photon systems. <i>Nature</i> , 2022, 606, 41-48.	13.7	66
15	Probing phonon dynamics with multidimensional high harmonic carrier-envelope-phase spectroscopy. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2022, 119, .	3.3	13
16	Frequency-Dependent Sternheimer Linear-Response Formalism for Strongly Coupled Light-Matter Systems. <i>Journal of Chemical Theory and Computation</i> , 2022, 18, 4354-4365.	2.3	9
17	Effect of spin-orbit coupling on the high harmonics from the topological Dirac semimetal Na <sub>3</sub> Bi. <i>Npj Computational Materials</i> , 2022, 8, .	3.5	13
18	Engineering quantum materials with chiral optical cavities. <i>Nature Materials</i> , 2021, 20, 438-442.	13.3	120



#	ARTICLE	IF	CITATIONS
37	The ferroelectric photo ground state of SrTiO <sub>3</sub> : Cavity materials engineering. Proceedings of the National Academy of Sciences of the United States of America, 2021, 118, .	3.3	49
38	Down-conversion processes in <i>ab initio</i> nonrelativistic quantum electrodynamics. Physical Review Research, 2021, 3, .	1.3	8
39	Out-of-Plane Transport of 1T-TaS <sub>2</sub> /Graphene-Based van der Waals Heterostructures. ACS Nano, 2021, 15, 11898-11907.	7.3	20
40	Approximations based on density-matrix embedding theory for density-functional theories. Electronic Structure, 2021, 3, 035001.	1.0	1
41	Quantum paraelectric phase of $\text{SrTiO}_3$ from first principles. Physical Review B, 2021, 104, .	2.1	1
42	Light-Driven Extremely Nonlinear Bulk Photogalvanic Currents. Physical Review Letters, 2021, 127, 126601.	2.9	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.	2.9	13
44	Engineering Three-Dimensional Moiré Flat Bands. Nano Letters, 2021, 21, 7519-7526.	4.5	10
45	Moiré correlations in ABCA graphene. Proceedings of the National Academy of Sciences of the United States of America, 2021, 118, .	3.3	59
46	Polaritonic Chemistry: Collective Strong Coupling Implies Strong Local Modification of Chemical Properties. Journal of Physical Chemistry Letters, 2021, 12, 508-516.	2.1	65
47	Realization of nearly dispersionless bands with strong orbital anisotropy from destructive interference in twisted bilayer MoS <sub>2</sub> . Nature Communications, 2021, 12, 5644.	5.8	57
48	Making <i>ab initio</i> QED functional(s): Nonperturbative and photon-free effective frameworks for strong light-matter coupling. Proceedings of the National Academy of Sciences of the United States of America, 2021, 118, .	3.3	42
49	Conditional Wave Function Theory: A Unified Treatment of Molecular Structure and Nonadiabatic Dynamics. Journal of Chemical Theory and Computation, 2021, , .	2.3	1
50	Common microscopic origin of the phase transitions in Ta <sub>2</sub> NiS <sub>5</sub> and the excitonic insulator candidate Ta <sub>2</sub> NiSe <sub>5</sub> . Npj Computational Materials, 2021, 7, .	3.5	19
51	Photoionization and transient Wannier-Stark ladder in silicon: First-principles simulations versus Keldysh theory. Physical Review B, 2021, 104, .	1.1	7
52	Entangled photon assisted multidimensional nonlinear optics of exciton polaritons. Journal of Applied Physics, 2020, 128, 113102.	1.1	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, .	2.8	29
54	Parameter-free hybridlike functional based on an extended Hubbard model: $\text{DFT} + \text{U}$ . Physical Review B, 2020, 102, .	1.2	1

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55	Dynamical amplification of electric polarization through nonlinear phononics in 2D SnTe. Npj Computational Materials, 2020, 6, .	3.5	12
56	Charge-Transfer Plasmon Polaritons at Graphene/ $\sqrt{1\pm}$ -RuCl <sub>3</sub> Interfaces. Nano Letters, 2020, 20, 8438-8445.	4.5	53
57	Light-Matter Hybrid-Orbital-Based First-Principles Methods: The Influence of Polariton Statistics. Journal of Chemical Theory and Computation, 2020, 16, 5601-5620.	2.3	19
58	Exact exchange-correlation potential of effectively interacting Kohn-Sham systems. Physical Review A, 2020, 101, .	1.0	1
59	Effect of many modes on self-polarization and photochemical suppression in cavities. Journal of Chemical Physics, 2020, 153, 104103.	1.2	44
60	Direct Measurement of Electron-Phonon Coupling with Time-Resolved ARPES. Physical Review Letters, 2020, 125, 136401.	2.9	27
61	Virial Relations for Electrons Coupled to Quantum Field Modes. Journal of Chemical Theory and Computation, 2020, 16, 6236-6243.	2.3	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.	2.1	26
63	Giant Exciton Mott Density in Anatase $\langle \text{mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"} \rangle \langle \text{mml:mrow} \rangle \langle \text{mml:msub} \rangle \langle \text{mml:mrow} \rangle \langle \text{mml:mi} \rangle \text{TiO} \langle / \text{mml:mi} \rangle \langle / \text{mml:mrow} \rangle \langle \text{mml:mrow} \rangle \langle \text{mml:mn} \rangle 2 \langle / \text{mml:mn} \rangle \langle / \text{mml:mrow} \rangle \langle / \text{mml:math} \rangle$ . Physical Review Letters, 2020, 125, 116403.	2.9	73
64	Coupled Cluster Theory for Molecular Polaritons: Changing Ground and Excited States. Physical Review X, 2020, 10, .	2.8	102
65	Ultrafast transient absorption spectroscopy of the charge-transfer insulator NiO: Beyond the dynamical Franz-Keldysh effect. Physical Review B, 2020, 102, .	1.1	12
66	Nature of Symmetry Breaking at the Excitonic Insulator Transition: $\langle \text{mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"} \rangle \langle \text{mml:mrow} \rangle \langle \text{mml:msub} \rangle \langle \text{mml:mrow} \rangle \langle \text{mml:mi} \rangle \text{Ta} \langle / \text{mml:mi} \rangle \langle / \text{mml:mrow} \rangle \langle \text{mml:mrow} \rangle \langle \text{mml:mn} \rangle 2 \langle / \text{mml:mn} \rangle \langle / \text{mml:mrow} \rangle \langle / \text{mml:math} \rangle$ . Physical Review Letters, 2020, 124, 197601.	2.9	73
67	Correlated electronic phases in twisted bilayer transition metal dichalcogenides. Nature Materials, 2020, 19, 861-866.	13.3	544
68	Room Temperature Terahertz Electroabsorption Modulation by Excitons in Monolayer Transition Metal Dichalcogenides. Nano Letters, 2020, 20, 5214-5220.	4.5	14
69	Polycyclic aromatic chains on metals and insulating layers by repetitive [3+2] Cycloadditions. Nature Communications, 2020, 11, 1490.	5.8	23
70	Electron-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.	3.3	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.	1.2	210
72	Local Berry curvature signatures in dichroic angle-resolved photoelectron spectroscopy from two-dimensional materials. Science Advances, 2020, 6, eaay2730.	4.7	57

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73	Setting the photoelectron clock through molecular alignment. <i>Nature Communications</i> , 2020, 11, 2546.	5.8	26
74	Universal slow plasmons and giant field enhancement in atomically thin quasi-two-dimensional metals. <i>Nature Communications</i> , 2020, 11, 1013.	5.8	53
75	Relevance of the Quadratic Diamagnetic and Self-Polarization Terms in Cavity Quantum Electrodynamics. <i>ACS Photonics</i> , 2020, 7, 975-990.	3.2	105
76	Covalent C-N Bond Formation through a Surface Catalyzed Thermal Cyclodehydrogenation. <i>Journal of the American Chemical Society</i> , 2020, 142, 3696-3700.	6.6	27
77	High-harmonic generation from spin-polarised defects in solids. <i>Npj Computational Materials</i> , 2020, 6, .	3.5	48
78	Polaritonic coupled-cluster theory. <i>Physical Review Research</i> , 2020, 2, .	1.3	57
79	Polariton panorama. <i>Nanophotonics</i> , 2020, 10, 549-577.	2.9	155
80	Light-induced topological magnons in two-dimensional van der Waals magnets. <i>SciPost Physics</i> , 2020, 9, .	1.5	18
81	Role of electron scattering on the high-order harmonic generation from solids. <i>Physical Review Research</i> , 2020, 2, .	1.3	3
82	Electronic Structure of Materials by Ab Initio Methods: Overview. , 2020, , 207-212.		0
83	Quantum Electrodynamical Bloch Theory with Homogeneous Magnetic Fields. <i>Physical Review Letters</i> , 2019, 123, 047202.	2.9	30
84	Maximized electron interactions at the magic angle in twisted bilayer graphene. <i>Nature</i> , 2019, 572, 95-100.	13.7	644
85	Multiflat Bands and Strong Correlations in Twisted Bilayer Boron Nitride: Doping-Induced Correlated Insulator and Superconductor. <i>Nano Letters</i> , 2019, 19, 4934-4940.	4.5	123
86	Integration of CLIP experiments of RNA-binding proteins: a novel approach to predict context-dependent splicing factors from transcriptomic data. <i>BMC Genomics</i> , 2019, 20, 521.	1.2	4
87	Force balance approach for advanced approximations in density functional theories. <i>Journal of Chemical Physics</i> , 2019, 151, 154107.	1.2	17
88	Self-Consistent Density-Functional Embedding: A Novel Approach for Density-Functional Approximations. <i>Journal of Chemical Theory and Computation</i> , 2019, 15, 5209-5220.	2.3	14
89	Reduced Density-Matrix Approach to Strong Matter-Photon Interaction. <i>ACS Photonics</i> , 2019, 6, 2694-2711.	3.2	31
90	Light-Matter Response in Nonrelativistic Quantum Electrodynamics. <i>ACS Photonics</i> , 2019, 6, 2757-2778.	3.2	79

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91	Capturing vacuum fluctuations and photon correlations in cavity quantum electrodynamics with multitrajjectory Ehrenfest dynamics. <i>Physical Review A</i> , 2019, 99, .	1.0	33
92	Cavity Control of Excitons in Two-Dimensional Materials. <i>Nano Letters</i> , 2019, 19, 3473-3479.	4.5	65
93	Density-Matrix Embedding Theory Study of the One-Dimensional Hubbardâ€“Holstein Model. <i>Journal of Chemical Theory and Computation</i> , 2019, 15, 2221-2232.	2.3	22
94	Orbital magneto-optical response of periodic insulators from first principles. <i>Npj Computational Materials</i> , 2019, 5, .	3.5	5
95	Modification of excitation and charge transfer in cavity quantum-electrodynamical chemistry. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2019, 116, 4883-4892.	3.3	138
96	Unraveling materials Berry curvature and Chern numbers from real-time evolution of Bloch states. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2019, 116, 4135-4140.	3.3	20
97	Light-matter interactions within the Ehrenfestâ€“Maxwellâ€“Pauliâ€“Kohnâ€“Sham framework: fundamentals, implementation, and nano-optical applications. <i>Advances in Physics</i> , 2019, 68, 225-333.	35.9	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. <i>Science Advances</i> , 2019, 5, eaax2937.	4.7	28
100	Benchmarking semiclassical and perturbative methods for real-time simulations of cavity-bound emission and interference. <i>Journal of Chemical Physics</i> , 2019, 151, 244113.	1.2	37
101	Optimal control theory for quantum electrodynamics: an initial state problem. <i>European Physical Journal B</i> , 2019, 92, 1.	0.6	6
102	Upstream analysis of alternative splicing: a review of computational approaches to predict context-dependent splicing factors. <i>Briefings in Bioinformatics</i> , 2019, 20, 1358-1375.	3.2	53
103	Nonadiabatic quantum dynamics without potential energy surfaces. <i>Physical Review Materials</i> , 2019, 3, .	0.9	12
104	Topological Floquet engineering of twisted bilayer graphene. <i>Physical Review Research</i> , 2019, 1, .	1.3	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. <i>Nature Reviews Chemistry</i> , 2018, 2, .	13.8	182
107	Ab Initio Optimized Effective Potentials for Real Molecules in Optical Cavities: Photon Contributions to the Molecular Ground State. <i>ACS Photonics</i> , 2018, 5, 992-1005.	3.2	96
108	Propagators for the Time-Dependent Kohnâ€“Sham Equations: Multistep, Rungeâ€“Kutta, Exponential Rungeâ€“Kutta, and Commutator Free Magnus Methods. <i>Journal of Chemical Theory and Computation</i> , 2018, 14, 3040-3052.	2.3	69

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109	Atomic-like high-harmonic generation from two-dimensional materials. <i>Science Advances</i> , 2018, 4, eaao5207.	4.7	98
110	Phonon-driven spin-Floquet magneto-valleytronics in MoS <sub>2</sub> . <i>Nature Communications</i> , 2018, 9, 638.	5.8	86
111	Phonon Driven Floquet Matter. <i>Nano Letters</i> , 2018, 18, 1535-1542.	4.5	63
112	Light-matter interaction in the long-wavelength limit: no ground-state without dipole self-energy. <i>Journal of Physics B: Atomic, Molecular and Optical Physics</i> , 2018, 51, 034005.	0.6	132
113	Ab Initio Simulation of Attosecond Transient Absorption Spectroscopy in Two-Dimensional Materials. <i>Applied Sciences (Switzerland)</i> , 2018, 8, 1777.	1.3	19
114	All-optical nonequilibrium pathway to stabilising magnetic Weyl semimetals in pyrochlore iridates. <i>Nature Communications</i> , 2018, 9, 4452.	5.8	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. <i>Nanoscience and Technology</i> , 2018, , 159-178.	1.5	1
117	Special issue in honor of Eberhard K.U. Gross for his 65th birthday. <i>European Physical Journal B</i> , 2018, 91, 1.	0.6	0
118	<i>Ab initio</i> nonrelativistic quantum electrodynamics: Bridging quantum chemistry and quantum optics from weak to strong coupling. <i>Physical Review A</i> , 2018, 98, .	1.0	126
119	Multiple-orbital effects in laser-induced electron diffraction of aligned molecules. <i>Physical Review A</i> , 2018, 98, .	1.0	14
120	Comparison of RNA-seq and microarray platforms for splice event detection using a cross-platform algorithm. <i>BMC Genomics</i> , 2018, 19, 703.	1.2	20
121	High-harmonic generation from few-layer hexagonal boron nitride: Evolution from monolayer to bulk response. <i>Physical Review B</i> , 2018, 98, .	1.1	54
122	Ultrafast Modification of Hubbard $U$ in a Strongly Correlated Material: <i>Ab Initio</i> High-Harmonic Generation in NiO. <i>Physical Review Letters</i> , 2018, 121, 097402.	2.9	118
123	Coupled forward-backward trajectory approach for nonequilibrium electron-ion dynamics. <i>Physical Review B</i> , 2018, 97, .	1.1	12
124	Role of intraband transitions in photocarrier generation. <i>Physical Review B</i> , 2018, 98, .	1.1	26
125	Phonon-Driven Selective Modulation of Exciton Oscillator Strengths in Anatase TiO <sub>2</sub> Nanoparticles. <i>Nano Letters</i> , 2018, 18, 5007-5014.	4.5	29
126	Kinetic-Energy Density-Functional Theory on a Lattice. <i>Journal of Chemical Theory and Computation</i> , 2018, 14, 4072-4087.	2.3	7



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127	First-principles simulations for attosecond photoelectron spectroscopy based on time-dependent density functional theory. <i>European Physical Journal B</i> , 2018, 91, 1.	0.6	15
128	Electronic Structure of Materials by Ab Initio Methods: Overview. , 2018, , 1-6.		0
129	Light-matter interactions via the exact factorization approach. <i>European Physical Journal B</i> , 2018, 91, 1.	0.6	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	0.1	20
131	Emergent elemental two-dimensional materials beyond graphene. <i>Journal Physics D: Applied Physics</i> , 2017, 50, 053004.	1.3	74
132	Creating stable Floquet-Weyl semimetals by laser-driving of 3D Dirac materials. <i>Nature Communications</i> , 2017, 8, 13940.	5.8	255
133	Ab initio Modelling of Plasmons in Metal-semiconductor Bilayer Transition-metal Dichalcogenide Heterostructures. <i>Israel Journal of Chemistry</i> , 2017, 57, 540-546.	1.0	4
134	Atoms and molecules in cavities, from weak to strong coupling in quantum-electrodynamics (QED) chemistry. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2017, 114, 3026-3034.	3.3	389
135	Impact of the Electronic Band Structure in High-Harmonic Generation Spectra of Solids. <i>Physical Review Letters</i> , 2017, 118, 087403.	2.9	226
136	Efficient and accurate modeling of electron photoemission in nanostructures with TDDFT. <i>European Physical Journal B</i> , 2017, 90, 1.	0.6	32
137	New Middle Pleistocene hominin cranium from Gruta da Aroeira (Portugal). <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2017, 114, 3397-3402.	3.3	81
138	Cavity Born-Oppenheimer Approximation for Correlated Electron-Nuclear-Photon Systems. <i>Journal of Chemical Theory and Computation</i> , 2017, 13, 1616-1625.	2.3	133
139	A First-Principles Time-Dependent Density Functional Theory Framework for Spin and Time-Resolved Angular-Resolved Photoelectron Spectroscopy in Periodic Systems. <i>Journal of Chemical Theory and Computation</i> , 2017, 13, 265-273.	2.3	49
140	Ellipticity dependence of high-harmonic generation in solids originating from coupled intraband and interband dynamics. <i>Nature Communications</i> , 2017, 8, 745.	5.8	146
141	Modeling of laser-pulse induced water decomposition on two-dimensional materials by simulations based on time-dependent density functional theory. <i>Physical Review B</i> , 2017, 96, .	1.1	20
142	Anomalous anisotropic exciton temperature dependence in rutile $\text{TiO}_2$ . <i>Physical Review B</i> , 2017, 96, .	1.1	18
143	TDDFT-Based Study on the Proton-DNA Collision. <i>Journal of Physical Chemistry B</i> , 2017, 121, 7276-7283.	1.2	8
144	Introduction to the Physics of Silicene and other 2D Materials. <i>Lecture Notes in Physics</i> , 2017, , .	0.3	33

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145	A Brief History of Silicene. Lecture Notes in Physics, 2017, , 1-11.	0.3	0
146	Freestanding Silicene. Lecture Notes in Physics, 2017, , 13-39.	0.3	3
147	Multilayer Silicene. Lecture Notes in Physics, 2017, , 53-61.	0.3	0
148	Germanene, Stanene and Other 2D Materials. Lecture Notes in Physics, 2017, , 63-85.	0.3	4
149	Bimodal supramolecular functionalization of carbon nanotubes triggered by covalent bond formation. Chemical Science, 2017, 8, 1927-1935.	3.7	29
150	Self-consistent $\langle \text{mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"} \rangle \langle \text{mml:mi mathvariant="normal"} \rangle \text{DFT} \langle \text{mml:mi} \rangle \langle \text{mml:mo} \rangle + \langle \text{mml:mo} \rangle \langle \text{mml:mi} \rangle \text{U} \langle \text{mml:mi} \rangle \langle \text{mml:math} \rangle$ method for real-space time-dependent density functional theory calculations. Physical Review B, 2017, 96, .	1.1	35
151	Exact functionals for correlated electronâ€“photon systems. New Journal of Physics, 2017, 19, 113036.	1.2	19
152	Electronic band gaps of confined linear carbon chains ranging from polyynes to carbynes. Physical Review Materials, 2017, 1, .	0.9	61
153	Exact maps in density functional theory for lattice models. New Journal of Physics, 2016, 18, 083004.	1.2	13
154	Universal steps in quantum dynamics with time-dependent potential-energy surfaces: Beyond the Born-Oppenheimer picture. Physical Review A, 2016, 94, .	1.0	10
155	Negative plasmon dispersion in $2\langle i \rangle \text{H} \langle /i \rangle \text{-NbS} \langle \text{sub} \rangle 2 \langle / \text{sub} \rangle$ beyond the charge-density-wave interpretation. New Journal of Physics, 2016, 18, 103050.	1.2	10
156	Tailored pump-probe transient spectroscopy with time-dependent density-functional theory: controlling absorption spectra. European Physical Journal B, 2016, 89, 1.	0.6	17
157	Confined linear carbon chains as a route to bulkâ€“carbyne. Nature Materials, 2016, 15, 634-639.	13.3	341
158	The mechanical bond on carbon nanotubes: diameter-selective functionalization and effects on physical properties. Nanoscale, 2016, 8, 9254-9264.	2.8	33
159	Imaging single-molecule reaction intermediates stabilized by surface dissipation and entropy. Nature Chemistry, 2016, 8, 678-683.	6.6	130
160	Disentangling Vacancy Oxidation on Metallicity-Sorted Carbon Nanotubes. Journal of Physical Chemistry C, 2016, 120, 18316-18322.	1.5	8
161	Noncovalent Dimerization after Enediyne Cyclization on Au(111). Journal of the American Chemical Society, 2016, 138, 10963-10967.	6.6	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.	1.2	7

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163	A large-scale analysis of alternative splicing reveals a key role of QKI in lung cancer. <i>Molecular Oncology</i> , 2016, 10, 1437-1449.	2.1	60
164	Monitoring Electron-Photon Dressing in $WSe_2$ . <i>Nano Letters</i> , 2016, 16, 7993-7998.	4.5	64
165	Density functional theory study of the $f$ - $d$ phase transition in cerium: Role of electron correlation and $d$ -orbital localization. <i>Physical Review B</i> , 2016, 93, .	1.1	23
166	Polyne electronic and vibrational properties under environmental interactions. <i>Physical Review B</i> , 2016, 94, .	1.1	45
167	Systematic construction of density functionals based on matrix product state computations. <i>New Journal of Physics</i> , 2016, 18, 083039.	1.2	16
168	On the Exciton Coupling between Two Chlorophyll Pigments in the Absence of a Protein Environment: Intrinsic Effects Revealed by Theory and Experiment. <i>Angewandte Chemie</i> , 2016, 128, 6356-6359.	1.6	4
169	Quantum plasmonics: from jellium models to ab initio calculations. <i>Nanophotonics</i> , 2016, 5, 409-426.	2.9	116
170	Electronic Structure of Low-Dimensional Carbon $\pi$ -Systems. <i>Journal of Physical Chemistry C</i> , 2016, 120, 12362-12368.	1.5	0
171	On the Exciton Coupling between Two Chlorophyll Pigments in the Absence of a Protein Environment: Intrinsic Effects Revealed by Theory and Experiment. <i>Angewandte Chemie - International Edition</i> , 2016, 55, 6248-6251.	7.2	19
172	Photoinduced Absorption within Single-Walled Carbon Nanotube Systems. <i>Journal of Physical Chemistry C</i> , 2016, 120, 1926-1935.	1.5	12
173	Static correlation and electron localization in molecular dimers from the self-consistent RPA and $G$ - $W$ . <i>Physical Review B</i> , 2015, 91, .	1.1	54
174	Optimized Effective Potential for Quantum Electrodynamical Time-Dependent Density Functional Theory. <i>Physical Review Letters</i> , 2015, 115, 093001.	2.9	93
175	Engineering Photophenomena in Large, 3D Structures Composed of Self-Assembled van der Waals Heterostructure Flakes. <i>Advanced Optical Materials</i> , 2015, 3, 1551-1556.	3.6	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?. <i>Journal of Physical Chemistry A</i> , 2015, 119, 11498-11503.	1.1	13
178	Kohn-Sham approach to quantum electrodynamical density-functional theory: Exact time-dependent effective potentials in real space. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2015, 112, 15285-15290.	3.3	107
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