Jeffrey B Neaton

List of Publications by Year
in descending order

Source: https://exaly.com/author-pdf/1237830/publications.pdf

Version: 2024-02-01

256 papers	31,229 citations	4658 85 h-index	4432 172 g-index
261 all docs	261 docs citations	261 times ranked	30097 citing authors

#	Article	IF	Citations
1	Epitaxial BiFeO3 Multiferroic Thin Film Heterostructures. Science, 2003, 299, 1719-1722.	12.6	5,548
2	First-principles study of metal adatom adsorption on graphene. Physical Review B, 2008, 77, .	3.2	1,245
3	First-principles study of spontaneous polarization in multiferroicBiFeO3. Physical Review B, 2005, 71, .	3.2	1,225
4	Cooperative insertion of CO2 in diamine-appended metal-organic frameworks. Nature, 2015, 519, 303-308.	27.8	1,026
5	Synthesis, Characterization, and Theory of [9]-, [12]-, and [18]Cycloparaphenylene: Carbon Nanohoop Structures. Journal of the American Chemical Society, 2008, 130, 17646-17647.	13.7	812
6	Renormalization of Molecular Electronic Levels at Metal-Molecule Interfaces. Physical Review Letters, 2006, 97, 216405.	7.8	769
7	Mechanically controlled binary conductance switching of a single-molecule junction. Nature Nanotechnology, 2009, 4, 230-234.	31.5	609
8	Software for the frontiers of quantum chemistry: An overview of developments in the Q-Chem 5 package. Journal of Chemical Physics, 2021, 155, 084801.	3.0	518
9	Elastic Properties of Chemical-Vapor-Deposited Monolayer MoS₂, WS₂, and Their Bilayer Heterostructures. Nano Letters, 2014, 14, 5097-5103.	9.1	512
10	Amineâ^'Gold Linked Single-Molecule Circuits:â€‰ Experiment and Theory. Nano Letters, 2007, 7, 3477-3482.	9.1	447
11	Pairing in dense lithium. Nature, 1999, 400, 141-144.	27.8	375
12	Single-molecule diodes with high rectification ratios through environmental control. Nature Nanotechnology, 2015, 10, 522-527.	31.5	360
13	Comprehensive study of carbon dioxide adsorption in the metalâ€"organic frameworks M₂(dobdc) (M = Mg, Mn, Fe, Co, Ni, Cu, Zn). Chemical Science, 2014, 5, 4569-4581.	7.4	342
14	Extrinsic models for the dielectric response of CaCu3Ti4O12. Journal of Applied Physics, 2003, 94, 3299-3306.	2.5	324
15	First-principles study of the structure and lattice dielectric response ofCaCu3Ti4O12. Physical Review B, 2002, 65, .	3.2	317
16	Theory and computation of hot carriers generated by surface plasmon polaritons in noble metals. Nature Communications, 2015, 6, 7044.	12.8	317
17	Theory of polarization enhancement in epitaxial BaTiO3/SrTiO3 superlattices. Applied Physics Letters, 2003, 82, 1586-1588.	3.3	316
18	Layered Halide Double Perovskites: Dimensional Reduction of Cs₂AgBiBr₆. Journal of the American Chemical Society, 2018, 140, 5235-5240.	13.7	293

#	Article	IF	Citations
19	Defect-Induced Band-Edge Reconstruction of a Bismuth-Halide Double Perovskite for Visible-Light Absorption. Journal of the American Chemical Society, 2017, 139, 5015-5018.	13.7	288
20	GW100: Benchmarking G₀W₀ for Molecular Systems. Journal of Chemical Theory and Computation, 2015, 11, 5665-5687.	5.3	280
21	Electron delocalization and charge mobility as a function of reduction in a metalâ€“organic framework. Nature Materials, 2018, 17, 625-632.	27.5	255
22	Simultaneous Determination of Conductance and Thermopower of Single Molecule Junctions. Nano Letters, 2012, 12, 354-358.	9.1	251
23	Cooperative carbon capture and steam regeneration with tetraamine-appended metalâ€“organic frameworks. Science, 2020, 369, 392-396.	12.6	249
24	Small-Molecule Adsorption in Open-Site Metalâ€“Organic Frameworks: A Systematic Density Functional Theory Study for Rational Design. Chemistry of Materials, 2015, 27, 668-678.	6.7	248
25	Gap renormalization of molecular crystals from density-functional theory. Physical Review B, 2013, 88, .	3.2	239
26	Quasiparticle Spectra from a Nonempirical Optimally Tuned Range-Separated Hybrid Density Functional. Physical Review Letters, 2012, 109, 226405.	7.8	236
27	Atomate: A high-level interface to generate, execute, and analyze computational materials science workflows. Computational Materials Science, 2017, 139, 140-152.	3.0	223
28	Ab initiostudy of the phase diagram of epitaxialBaTiO3. Physical Review B, 2004, 69, .	3.2	217
29	Reversible CO Binding Enables Tunable CO/H₂ and CO/N₂ Separations in Metalâ€“Organic Frameworks with Exposed Divalent Metal Cations. Journal of the American Chemical Society, 2014, 136, 10752-10761.	13.7	210
30	Solid-state optical absorption from optimally tuned time-dependent range-separated hybrid density functional theory. Physical Review B, 2015, 92, .	3.2	210
31	Charge density wave order in 1D mirror twin boundaries of single-layer MoSe2. Nature Physics, 2016, 12, 751-756.	16.7	209
32	The Mechanism of Carbon Dioxide Adsorption in an Alkylamine-Functionalized Metalâ€“Organic Framework. Journal of the American Chemical Society, 2013, 135, 7402-7405.	13.7	208
33	AbÂInitioStudy of Hot Carriers in the First Picosecond after Sunlight Absorption in Silicon. Physical Review Letters, 2014, 112, 257402.	7.8	203
34	Non-chemisorbed goldâ€“sulfur binding prevails in self-assembled monolayers. Nature Chemistry, 2019, 11, 351-358.	13.6	202
35	Enrichment of molecular antenna triplets amplifies upconverting nanoparticle emission. Nature Photonics, 2018, 12, 402-407.	31.4	200
36	Identifying substitutional oxygen as a prolific point defect in monolayer transition metal dichalcogenides. Nature Communications, 2019, 10, 3382.	12.8	196

#	Article	IF	Citations
37	Inversion symmetry and bulk Rashba effect in methylammonium lead iodide perovskite single crystals. Nature Communications, 2018, 9, 1829.	12.8	189
38	Conductance and Geometry of Pyridine-Linked Single-Molecule Junctions. Journal of the American Chemical Society, 2010, 132, 6817-6821.	13.7	186
39	Large Bulk Photovoltaic Effect and Spontaneous Polarization of Single-Layer Monochalcogenides. Physical Review Letters, 2017, 119, 067402.	7.8	182
40	Quasiparticle and optical spectroscopy of the organic semiconductors pentacene and PTCDA from first principles. Physical Review B, 2012, 85, .	3.2	181
41	Tunability of the dielectric response of epitaxially strainedSrTiO3from first principles. Physical Review B, 2005, 71, .	3.2	178
42	Tuning Rectification in Single-Molecular Diodes. Nano Letters, 2013, 13, 6233-6237.	9.1	169
43	Low-Energy Charge-Transfer Excitons in Organic Solids from First-Principles: The Case of Pentacene. Journal of Physical Chemistry Letters, 2013, 4, 2197-2201.	4.6	166
44	Structural, electronic, and magnetic properties ofSrRuO3under epitaxial strain. Physical Review B, 2006, 74, .	3.2	162
45	Negative Differential Resistance in Carbon Atomic Wire-Carbon Nanotube Junctions. Nano Letters, 2008, 8, 2900-2905.	9.1	160
46	Design of a Metalâ€“Organic Framework with Enhanced Back Bonding for Separation of N₂ and CH₄. Journal of the American Chemical Society, 2014, 136, 698-704.	13.7	157
47	Solar fuels photoanode materials discovery by integrating high-throughput theory and experiment. Proceedings of the National Academy of Sciences of the United States of America, 2017, 114, 3040-3043.	7.1	157
48	Length Dependence of Conductance in Aromatic Single-Molecule Junctions. Nano Letters, 2009, 9, 3949-3953.	9.1	151
49	On the Constitution of Sodium at Higher Densities. Physical Review Letters, 2001, 86, 2830-2833.	7.8	145
50	Detection of sub-MeV dark matter with three-dimensional Dirac materials. Physical Review D, 2018, 97, .	4.7	142
51	Understanding Trends in CO₂ Adsorption in Metalâ€“Organic Frameworks with Open-Metal Sites. Journal of Physical Chemistry Letters, 2014, 5, 861-865.	4.6	139
52	molgw 1: Many-body perturbation theory software for atoms, molecules, and clusters. Computer Physics Communications, 2016, 208, 149-161.	7.5	139
53	A systematic benchmark of the ab initio Bethe-Salpeter equation approach for low-lying optical excitations of small organic molecules. Journal of Chemical Physics, 2015, 142, 244101.	3.0	137
54	Smallâ€Bandâ€Gap Halide Double Perovskites. Angewandte Chemie - International Edition, 2018, 57, 12765-12770.	13.8	136

#	Article	IF	Citations
55	Charge Separation via Strain in Silicon Nanowires. Nano Letters, 2009, 9, 2418-2422.	9.1	131
56	Excited-state vibrational dynamics toward the polaron in methylammonium lead iodide perovskite. Nature Communications, 2018, 9, 2525.	12.8	129
57	Outer-valence Electron Spectra of Prototypical Aromatic Heterocycles from an Optimally Tuned Range-Separated Hybrid Functional. Journal of Chemical Theory and Computation, 2014, 10, 1934-1952.	5.3	128
58	First-principles study of symmetry lowering and polarization inBaTiO3âˆ•SrTiO3superlattices with in-plane expansion. Physical Review B, 2005, 71, .	3.2	127
59	Band Gap and Edge Engineering via Ferroic Distortion and Anisotropic Strain: The Case of<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:msub><mml:mi>SrTiO</mml:mi><mml:mn>3</mml:mn></mml:msub></mml:math>. Physical Review Letters, 2011, 107, 146804.	7.8	124
60	Tuning Semiconductor Band Edge Energies for Solar Photocatalysis via Surface Ligand Passivation. Nano Letters, 2012, 12, 383-388.	9.1	124
61	Chemical Raman Enhancement of Organic Adsorbates on Metal Surfaces. Physical Review Letters, 2011, 106, 083003.	7.8	123
62	Force-Field Development from Electronic Structure Calculations with Periodic Boundary Conditions: Applications to Gaseous Adsorption and Transport in Metalâ€“Organic Frameworks. Journal of Chemical Theory and Computation, 2014, 10, 1477-1488.	5.3	121
63	Determination of Energy Level Alignment and Coupling Strength in 4,4â€²-Bipyridine Single-Molecule Junctions. Nano Letters, 2014, 14, 794-798.	9.1	112
64	Reliable Energy Level Alignment at Physisorbed Moleculeâ€“Metal Interfaces from Density Functional Theory. Nano Letters, 2015, 15, 2448-2455.	9.1	112
65	Electronic Properties of theSi/SiO2Interface from First Principles. Physical Review Letters, 2000, 85, 1298-1301.	7.8	111
66	Defect-Induced Modification of Low-Lying Excitons and Valley Selectivity in Monolayer Transition Metal Dichalcogenides. Physical Review Letters, 2018, 121, 167402.	7.8	109
67	Formation of the layered conductive magnet CrCl2(pyrazine)2 through redox-active coordination chemistry. Nature Chemistry, 2018, 10, 1056-1061.	13.6	108
68	Tunable Charge Transport in Single-Molecule Junctions via Electrolytic Gating. Nano Letters, 2014, 14, 1400-1404.	9.1	107
69	Elucidating CO₂ Chemisorption in Diamine-Appended Metalâ€“Organic Frameworks. Journal of the American Chemical Society, 2018, 140, 18016-18031.	13.7	107
70	Water Enables Efficient CO₂ Capture from Natural Gas Flue Emissions in an Oxidation-Resistant Diamine-Appended Metalâ€“Organic Framework. Journal of the American Chemical Society, 2019, 141, 13171-13186.	13.7	107
71	Ab initio study of hot electrons in GaAs. Proceedings of the National Academy of Sciences of the United States of America, 2015, 112, 5291-5296.	7.1	104
72	Electric Field- and Strain-Induced Rashba Effect in Hybrid Halide Perovskites. Journal of Physical Chemistry Letters, 2016, 7, 3683-3689.	4.6	104

#	Article	IF	Citations
73	Environmental Control of Single-Molecule Junction Transport. Nano Letters, 2011, 11, 1988-1992.	9.1	103
74	Electronic Energy Levels of Weakly Coupled Nanostructures:<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:msub><mml:mi mathvariant="normal">C</mml:mi><mml:mn>60</mml:mn></mml:msub></mml:math>-Metal Interfaces. Physical Review Letters, 2008, 101, 026804.	7.8	102
75	Strain-Induced Band Gap Modification in Coherent Core/Shell Nanostructures. Nano Letters, 2010, 10, 3156-3162.	9.1	101
76	Manipulating magnetic properties of<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:msub><mml:mrow><mml:mtext>SrRuO</mml:mtext></mml:mrow><mml:mn>3</mml:mn></mml: xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:msub><mml:mrow><mml:mtext>CaRuO</mml:mtext></mml:mrow><mml:mn>3</mml:mn></mml: epitaxial and uniaxial strains. Physical Review B, 2008, 77, .	3.2	98
77	Relating Energy Level Alignment and Amine-Linked Single Molecule Junction Conductance. Nano Letters, 2010, 10, 2470-2474.	9.1	95
78	Ligand-Assisted Enhancement of CO₂ Capture in Metalâ€“Organic Frameworks. Journal of the American Chemical Society, 2012, 134, 6714-6719.	13.7	95
79	Charge transport and rectification in molecular junctions formed with carbon-based electrodes. Proceedings of the National Academy of Sciences of the United States of America, 2014, 111, 10928-10932.	7.1	95
80	Force Field Development from Periodic Density Functional Theory Calculations for Gas Separation Applications Using Metalâ€“Organic Frameworks. Journal of Physical Chemistry C, 2016, 120, 12590-12604.	3.1	95
81	A reversible single-molecule switch based on activated antiaromaticity. Science Advances, 2017, 3, eaao2615.	10.3	94
82	Lattice dielectric response ofCdCu3Ti4O12andCaCu3Ti4O12from first principles. Physical Review B, 2003, 67, .	3.2	93
83	CO2 Capture by Metalâ€“Organic Frameworks with van der Waals Density Functionals. Journal of Physical Chemistry A, 2012, 116, 4957-4964.	2.5	92
84	Beyond Energies: Geometries of Nonbonded Molecular Complexes as Metrics for Assessing Electronic Structure Approaches. Journal of Chemical Theory and Computation, 2015, 11, 1481-1492.	5.3	90
85	Molecular adsorption on metal surfaces with van der Waals density functionals. Physical Review B, 2012, 85, .	3.2	89
86	Structural and excited-state properties of oligoacene crystals from first principles. Physical Review B, 2016, 93, .	3.2	89
87	Excited-State Properties of Molecular Solids from First Principles. Annual Review of Physical Chemistry, 2016, 67, 587-616.	10.8	88
88	Thermopower of Amineâ^'Gold-Linked Aromatic Molecular Junctions from First Principles. ACS Nano, 2011, 5, 551-557.	14.6	87
89	Control of Single-Molecule Junction Conductance of Porphyrins via a Transition-Metal Center. Nano Letters, 2014, 14, 5365-5370.	9.1	83
90	High Throughput Discovery of Solar Fuels Photoanodes in the CuOâ€“V₂O₅ System. Advanced Energy Materials, 2015, 5, 1500968.	19.5	82

#	Article	IF	Citations
91	First-principles study of adhesion atCu/SiO2interfaces. Physical Review B, 2003, 68, .	3.2	81
92	An assessment of low-lying excitation energies and triplet instabilities of organic molecules with an ab initio Bethe-Salpeter equation approach and the Tamm-Dancoff approximation. Journal of Chemical Physics, 2017, 146, 194108.	3.0	81
93	Structural evidence for enhanced polarization in a commensurate short-period BaTiO3âˆ•SrTiO3 superlattice. Applied Physics Letters, 2006, 89, 092905.	3.3	80
94	Inverse Rectification in Donorâ€“Acceptor Molecular Heterojunctions. ACS Nano, 2011, 5, 9256-9263.	14.6	77
95	Relating the Physical Structure and Optoelectronic Function of Crystalline TIPSâ€Pentacene. Advanced Functional Materials, 2015, 25, 2038-2046.	14.9	77
96	Electronically Transparent Auâ€“N Bonds for Molecular Junctions. Journal of the American Chemical Society, 2017, 139, 14845-14848.	13.7	76
97	Electronic energy level alignment at metal-molecule interfaces with a<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>approach. Physical Review B, 2011, 84, .	3.2	75
98	First-principles Hubbard U approach for small molecule binding in metal-organic frameworks. Journal of Chemical Physics, 2016, 144, 174104.	3.0	73
99	Quantitative Currentâ€“Voltage Characteristics in Molecular Junctions from First Principles. Nano Letters, 2012, 12, 6250-6254.	9.1	72
100	Quantum Confinement and Electronic Properties of Tapered Silicon Nanowires. Physical Review Letters, 2008, 100, 246804.	7.8	71
101	Electronic level alignment at a metal-molecule interface from a short-range hybrid functional. Journal of Chemical Physics, 2011, 135, 164706.	3.0	71
102	Evaluating the GW Approximation with CCSD(T) for Charged Excitations Across the Oligoacenes. Journal of Chemical Theory and Computation, 2016, 12, 2834-2842.	5.3	71
103	Assessing DFT-D3 Damping Functions Across Widely Used Density Functionals: Can We Do Better?. Journal of Chemical Theory and Computation, 2017, 13, 2043-2052.	5.3	71
104	Computational design of low-band-gap double perovskites. Physical Review B, 2012, 86, .	3.2	70
105	Long-Lived Correlated Triplet Pairs in a Ï€-Stacked Crystalline Pentacene Derivative. Journal of the American Chemical Society, 2018, 140, 2326-2335.	13.7	68
106	Epitaxial growth of multiferroic YMnO3 on GaN. Applied Physics Letters, 2005, 87, 171915.	3.3	67
107	Voltage tuning of vibrational mode energies in single-molecule junctions. Proceedings of the National Academy of Sciences of the United States of America, 2014, 111, 1282-1287.	7.1	63
108	Low-Lying Electronic Excited States of Pentacene Oligomers: A Comparative Electronic Structure Study in the Context of Singlet Fission. Journal of Chemical Theory and Computation, 2015, 11, 147-156.	5.3	63

#	Article	IF	Citations
109	Mechanical and Charge Transport Properties of Alkanethiol Self-Assembled Monolayers on a Au(111) Surface:â€‰ The Role of Molecular Tilt. Langmuir, 2008, 24, 2219-2223.	3.5	62
110	Mn₂V₂O₇: An Earth Abundant Light Absorber for Solar Water Splitting. Advanced Energy Materials, 2015, 5, 1401840.	19.5	61
111	Comparing time-dependent density functional theory with many-body perturbation theory for semiconductors: Screened range-separated hybrids and the <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 plus Bethe-Salpeter approach. Physical Review Materials, 2019, 3, .	2.4	61
112	Low-Energy Linear Structures in Dense Oxygen: Implications for theÎµPhase. Physical Review Letters, 2002, 88, 205503.	7.8	59
113	Energy level alignment at molecule-metal interfaces from an optimally tuned range-separated hybrid functional. Journal of Chemical Physics, 2017, 146, .	3.0	59
114	Mapping the Transmission Functions of Single-Molecule Junctions. Nano Letters, 2016, 16, 3949-3954.	9.1	58
115	Tuning the bandgap of Cs₂AgBiBr₆ through dilute tin alloying. Chemical Science, 2019, 10, 10620-10628.	7.4	58
116	Cooperative Carbon Dioxide Adsorption in Alcoholamineâ€•and Alkoxyalkylamineâ€Functionalized Metalâ€“Organic Frameworks. Angewandte Chemie - International Edition, 2020, 59, 19468-19477.	13.8	58
117	Carrier Diffusion Lengths Exceeding 1 Î¼m Despite Trap-Limited Transport in Halide Double Perovskites. ACS Energy Letters, 2020, 5, 1337-1345.	17.4	58
118	Directed assembly of layered perovskite heterostructures as single crystals. Nature, 2021, 597, 355-359.	27.8	58
119	Probing Adsorption Interactions in Metalâ€“Organic Frameworks using X-ray Spectroscopy. Journal of the American Chemical Society, 2013, 135, 18183-18190.	13.7	56
120	Stability and self-passivation of copper vanadate photoanodes under chemical, electrochemical, and photoelectrochemical operation. Physical Chemistry Chemical Physics, 2016, 18, 9349-9352.	2.8	56
121	Solar fuel photoanodes prepared by inkjet printing of copper vanadates. Journal of Materials Chemistry A, 2016, 4, 7483-7494.	10.3	56
122	Ab initioelectronic relaxation times and transport in noble metals. Physical Review B, 2016, 94, .	3.2	56
123	Dirac metal to topological metal transition at a structural phase change in<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:msub><mml:mrow><mml:mi mathvariant="normal">Au</mml:mi></mml:mrow><mml:mn>2</mml:mn></mml:msub><mml:mi mathvariant="normal">Pb</mml:mi></mml:math>and prediction of<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:msub><mml:mrow><mml:mi mathvariant="double-struck">Z</mml:mi></mml:mrow><mml:mn>2</mml:mn></mml:msub></mml:math>topology	3.2	55
124	Origins of Singlet Fission in Solid Pentacene from an abÂinitio Greenâ€™s Function Approach. Physical Review Letters, 2017, 119, 267401.	7.8	55
125	Room-temperature skyrmion lattice in a layered magnet (Fe _{0.5} Co _{0.5}) ₅ GeTe ₂. Science Advances, 2022, 8, eabm7103.	10.3	55
126	Negative Differential Resistance in Transport through Organic Molecules on Silicon. Physical Review Letters, 2007, 98, 066807.	7.8	54

#	Article	IF	Citations
127	Observation of a two-dimensional Fermi surface and Dirac dispersion in <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:msub><mml:mi>YbMnSb</mml:mi><mml:mn>2</mml:mn></mml:msub> Physical Review B, 2018, 97, .	3.2	54
128	Density functional theory based calculation of small-polaron mobility in hematite. Physical Review B, 2014, 89, .	3.2	53
129	Quantitative molecular orbital energies within a G0W0 approximation. European Physical Journal B, 2012, 85, 1.	1.5	52
130	Effect of reduced dimensionality on the optical band gap of SrTiO3. Applied Physics Letters, 2013, 102, .	3.3	52
131	Controlling the Thermoelectric Properties of Thiophene-Derived Single-Molecule Junctions. Chemistry of Materials, 2014, 26, 7229-7235.	6.7	52
132	Using Molecular Design to Control the Performance of Hydrogen-Producing Polymer-Brush-Modified Photocathodes. Journal of Physical Chemistry Letters, 2014, 5, 3222-3226.	4.6	52
133	Quantitative Prediction of Optical Absorption in Molecular Solids from an Optimally Tuned Screened Range-Separated Hybrid Functional. Journal of Chemical Theory and Computation, 2018, 14, 2919-2929.	5.3	51
134	Simultaneous Determination of Structures, Vibrations, and Frontier Orbital Energies from a Self-Consistent Range-Separated Hybrid Functional. Journal of Physical Chemistry Letters, 2014, 5, 2734-2741.	4.6	49
135	Band gaps of crystalline solids from Wannier-localizationâ€“based optimal tuning of a screened range-separated hybrid functional. Proceedings of the National Academy of Sciences of the United States of America, 2021, 118, .	7.1	49
136	Reducing Coercive-Field Scaling in Ferroelectric Thin Films via Orientation Control. ACS Nano, 2018, 12, 4736-4743.	14.6	47
137	Relating Trends in First-Principles Electronic Structure and Open-Circuit Voltage in Organic Photovoltaics. Journal of Physical Chemistry Letters, 2011, 2, 2531-2537.	4.6	45
138	CO₂ induced phase transitions in diamine-appended metalâ€“organic frameworks. Chemical Science, 2015, 6, 5177-5185.	7.4	45
139	Transferable pair potentials for CdS and ZnS crystals. Journal of Chemical Physics, 2012, 136, 234111.	3.0	44
140	Probing the mechanism of CO₂ capture in diamine-appended metalâ€“organic frameworks using measured and simulated X-ray spectroscopy. Physical Chemistry Chemical Physics, 2015, 17, 21448-21457.	2.8	43
141	Phonon Screening of Excitons in Semiconductors: Halide Perovskites and Beyond. Physical Review Letters, 2021, 127, 067401.	7.8	42
142	Push it to the limit: Characterizing the convergence of common sequences of basis sets for intermolecular interactions as described by density functional theory. Journal of Chemical Physics, 2016, 144, 194306.	3.0	41
143	Ab initiophonon dispersion in crystalline naphthalene using van der Waals density functionals. Physical Review B, 2016, 93, .	3.2	41
144	Performance of van der Waals Corrected Functionals for Guest Adsorption in the M₂(dobdc) Metalâ€“Organic Frameworks. Journal of Physical Chemistry A, 2017, 121, 4139-4151.	2.5	41

#	Article	IF	Citations
145	Interplay of Bias-Driven Charging and the Vibrational Stark Effect in Molecular Junctions. Nano Letters, 2016, 16, 1104-1109.	9.1	40
146	Parameter-free driven Liouville-von Neumann approach for time-dependent electronic transport simulations in open quantum systems. Journal of Chemical Physics, 2017, 146, 092331.	3.0	40
147	Effective empirical corrections for basis set superposition error in the def2-SVPD basis: gCP and DFT-C. Journal of Chemical Physics, 2017, 146, 234105.	3.0	39
148	Topological materials discovery using electron filling constraints. Nature Physics, 2018, 14, 55-61.	16.7	39
149	Enhancement of CO₂ binding and mechanical properties upon diamine functionalization of M₂(dobpdc) metalâ€“organic frameworks. Chemical Science, 2018, 9, 5197-5206.	7.4	39
150	An automatically curated first-principles database of ferroelectrics. Scientific Data, 2020, 7, 72.	5.3	39
151	Towards predictive band gaps for halide perovskites: Lessons from one-shot and eigenvalue self-consistent <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 Materials, 2019, 3, .	2.4	39
152	Formation of<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:msub><mml:mtext>Y</mml:mtext><mml:mn>2</mml:mn></mml:msub><mml:msub><mml:mtext> in nanostructured ferritic alloys during isothermal and anisothermal heat treatment: A kinetic Monte Carlo study. Physical Review B, 2009, 80, .	3.2	38
153	Probing Charge Transport through Peptide Bonds. Journal of Physical Chemistry Letters, 2018, 9, 763-767.	4.6	38
154	Nonperturbative Visualization of Nanoscale Plasmonic Field Distributions via Photon Localization Microscopy. Physical Review Letters, 2011, 106, 037402.	7.8	37
155	Structure and electronic properties of cerium orthophosphate: Theory and experiment. Physical Review B, 2011, 83, .	3.2	36
156	Discovery of Manganese-Based Solar Fuel Photoanodes via Integration of Electronic Structure Calculations, Pourbaix Stability Modeling, and High-Throughput Experiments. ACS Energy Letters, 2017, 2, 2307-2312.	17.4	36
157	Reproducibility in <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline" id="d1e1825" altimg="si271.svg"><mml:mrow><mml:msub><mml:mrow><mml:mi>G</mml:mi></mml:mrow><mml:mrow><mml:mn>0</mml:mn></ calculations for solids. Computer Physics Communications, 2020, 255, 107242.	7.5	36
158	Low-lying excited states in crystalline perylene. Proceedings of the National Academy of Sciences of the United States of America, 2018, 115, 284-289.	7.1	35
159	Expanded Analogs of Threeâ€Dimensional Leadâ€Halide Hybrid Perovskites. Angewandte Chemie - International Edition, 2020, 59, 19087-19094.	13.8	35
160	Pairing, Ï€-bonding, and the role of nonlocality in a dense lithium monolayer. Physical Review B, 2000, 62, 8494-8499.	3.2	34
161	Adsorption-Induced Solvent-Based Electrostatic Gating of Charge Transport through Molecular Junctions. Nano Letters, 2015, 15, 4498-4503.	9.1	34
162	Accelerating GW-Based Energy Level Alignment Calculations for Moleculeâ€“Metal Interfaces Using a Substrate Screening Approach. Journal of Chemical Theory and Computation, 2019, 15, 4218-4227.	5.3	34

#	Article	IF	Citations
163	Origins of the Pressure-Induced Phase Transition and Metallization in the Halide Perovskite (CH₃NH₃)PbI₃. ACS Energy Letters, 2020, 5, 2174-2181.	17.4	34
164	Understanding Smallâ€Molecule Interactions in Metalâ€“Organic Frameworks: Coupling Experiment with Theory. Advanced Materials, 2015, 27, 5785-5796.	21.0	33
165	Assessment of two hybrid van der Waals density functionals for covalent and non-covalent binding of molecules. Journal of Chemical Physics, 2017, 146, 234106.	3.0	33
166	Molecular-Scale Quantum Dots from Carbon Nanotube Heterojunctions. Nano Letters, 2009, 9, 1544-1548.	9.1	31
167	Chemically Localized Resonant Excitons in Silverâ€“Pnictogen Halide Double Perovskites. Journal of Physical Chemistry Letters, 2021, 12, 2057-2063.	4.6	31
168	Successes and Opportunities for Discovery of Metal Oxide Photoanodes for Solar Fuels Generators. ACS Energy Letters, 2020, 5, 1413-1421.	17.4	30
169	Theory of Covalent Adsorbate Frontier Orbital Energies on Functionalized Light-Absorbing Semiconductor Surfaces. Journal of Physical Chemistry Letters, 2013, 4, 1701-1706.	4.6	29
170	Fermi-crossing Type-II Dirac fermions and topological surface states in NiTe2. Scientific Reports, 2020, 10, 12957.	3.3	29
171	Harnessing Chemical Raman Enhancement for Understanding Organic Adsorbate Binding on Metal Surfaces. Journal of Physical Chemistry Letters, 2012, 3, 1357-1362.	4.6	26
172	Band gap renormalization, carrier mobilities, and the electron-phonon self-energy in crystalline naphthalene. Physical Review B, 2020, 101, .	3.2	26
173	Density of states prediction for materials discovery via contrastive learning from probabilistic embeddings. Nature Communications, 2022, 13, 949.	12.8	26
174	Nonlinear variations in the electronic structure of IIâ€“VI and IIIâ€“V wurtzite semiconductors with biaxial strain. Applied Physics Letters, 2011, 98, .	3.3	24
175	Effects of self-consistency and plasmon-pole models on<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:math>for closed-shell molecules. Physical Review B, 2014, 90, .	3.2	24
176	Voltage Dependence of Moleculeâ€“Electrode Coupling in Biased Molecular Junctions. Journal of Physical Chemistry C, 2017, 121, 21136-21144.	3.1	24
177	Screening of Excitons by Organic Cations in Quasi-Two-Dimensional Organicâ€“Inorganic Lead-Halide Perovskites. Nano Letters, 2022, 22, 4870-4878.	9.1	24
178	Efficient Determination of Accurate Force Fields for Porous Materials Using ab Initio Total Energy Calculations. Journal of Physical Chemistry C, 2014, 118, 2693-2701.	3.1	23
179	High Compressionâ€Induced Conductivity in a Layered Cuâ€“Br Perovskite. Angewandte Chemie - International Edition, 2020, 59, 4017-4022.	13.8	23
180	Mechanism for bias-assisted indium mass transport on carbon nanotube surfaces. Physical Review B, 2005, 72, .	3.2	22

#	Article	IF	Citations
181	Flat branches and pressure amorphization. Journal of Non-Crystalline Solids, 2002, 307-310, 602-612.	3.1	20
182	First-Principles Studies of the Dynamics of [2]Rotaxane Molecular Switches. Nano Letters, 2009, 9, 3225-3229.	9.1	20
183	Assessing electronic structure approaches for gas-ligand interactions in metal-organic frameworks: The CO2-benzene complex. Journal of Chemical Physics, 2014, 140, 104707.	3.0	20
184	A direct look at halogen bonds. Science, 2017, 358, 167-168.	12.6	20
185	Bi-Containing n-FeWO4 Thin Films Provide the Largest Photovoltage and Highest Stability for a Sub-2 eV Band Gap Photoanode. ACS Energy Letters, 2018, 3, 2769-2774.	17.4	20
186	Ferromagnetic instabilities in atomically thin lithium and sodium wires. International Journal of Quantum Chemistry, 2003, 91, 239-244.	2.0	19
187	Real-space pseudopotential calculations of spin-dependent electron transport in magnetic molecular junctions. Physical Review B, 2007, 76, .	3.2	19
188	Zigzag Inversion Domain Boundaries in Indium Zinc Oxide-Based Nanowires: Structure and Formation. ACS Nano, 2013, 7, 10747-10751.	14.6	19
189	Communication: Energy-dependent resonance broadening in symmetric and asymmetric molecular junctions from an ab initio non-equilibrium Green's function approach. Journal of Chemical Physics, 2014, 141, 131104.	3.0	19
190	Ytterbium-driven strong enhancement of electron-phonon coupling in graphene. Physical Review B, 2014, 90, .	3.2	19
191	Ligand Coupling Symmetry Correlates with Thermopower Enhancement in Small-Molecule/Nanocrystal Hybrid Materials. ACS Nano, 2014, 8, 10528-10536.	14.6	19
192	Thermodynamic signature of Dirac electrons across a possible topological transition in <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:msub><mml:mi>ZrTe</mml:mi><mml:mn>5</mml:mn></mml:msub></mml:math> Physical Review B, 2018, 97, .	3.2	19
193	Smallâ€Bandâ€Gap Halide Double Perovskites. Angewandte Chemie, 2018, 130, 12947-12952.	2.0	19
194	Reduced scaling formulation of CASPT2 analytical gradients using the supporting subspace method. Journal of Chemical Physics, 2021, 154, 014103.	3.0	19
195	Cooperative Gas Adsorption without a Phase Transition in Metal-Organic Frameworks. Physical Review Letters, 2018, 121, 015701.	7.8	17
196	Anisotropic 2D excitons unveiled in organicâ€“inorganic quantum wells. Materials Horizons, 2021, 8, 197-208.	12.2	17
197	Exchange Bias in a Layered Metalâ€“Organic Topological Spin Glass. ACS Central Science, 2021, 7, 1317-1326.	11.3	17
198	Thermoelectricity at the gate. Nature Nanotechnology, 2014, 9, 876-877.	31.5	16

#	Article	IF	Citations
199	Phosphonic Acid Adsorbates Tune the Surface Potential of TiO₂ in Gas and Liquid Environments. Journal of Physical Chemistry Letters, 2014, 5, 2450-2454.	4.6	15
200	Numerical integration for ab initio many-electron self energy calculations within the GW approximation. Journal of Computational Physics, 2015, 286, 1-13.	3.8	15
201	Competing Thermodynamic and Dynamic Factors Select Molecular Assemblies on a Gold Surface. Physical Review Letters, 2013, 111, 265701.	7.8	14
202	Effects of quantum confinement on excited state properties 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></m initio</i>many-body perturbation theory. Physical Review B, 2016, 94, .	3.2	14
203	Anisotropic Dirac Fermions in BaMnBi2 and BaZnBi2. Scientific Reports, 2018, 8, 15322.	3.3	14
204	Half-magnetization plateau and the origin of threefold symmetry breaking in an electrically switchable triangular antiferromagnet. Physical Review Research, 2020, 2, .	3.6	14
205	Highly Tunable Magnetic Phases in Transition-Metal Dichalcogenide <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:msub><mml:mrow><mml:mi>Fe</mml:mi></mml:mrow><mml:mrow><mml:mn>1</mml:mn><m stretchy="false">/</mml:mo><mml:mn>3</mml:mn><mml:mo>+</mml:mo><mml:mi>Î´</mml:mi></mml:mrow></mml:msub><mml:m Physical Review X, 2022, 12, .	8.9	14
206	First-principles study of electronic structure and photocatalytic properties of MnNiO₃ as an alkaline oxygen-evolution photocatalyst. Chemical Communications, 2015, 51, 2867-2870.	4.1	13
207	Enhanced polarization in strained BaTiO₃ from first principles. Materials Research Society Symposia Proceedings, 2002, 718, 1.	0.1	12
208	First-principles studies of the electronic structure of cyclopentene on Si(001): density functional theory and GW calculations. Physica Status Solidi (B): Basic Research, 2006, 243, 2048-2053.	1.5	12
209	Contact dependence of the conductance of<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:msub><mml:mi mathvariant="normal">H</mml:mi><mml:mn>2</mml:mn></mml:msub></mml:math>molecular junctions from first principles. Physical Review B, 2008, 77, .	3.2	12
210	Origins of anisotropic transport in the electrically switchable antiferromagnet <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:msub><mml:mrow><mml:mi>Fe</mml:mi></mml:mrow><mml:mrow><mml:mn Physical Review B, 2021, 103, .	3.2	12
211	First-principles description of phonons inNi50Pt50disordered alloys:â€‚The role of relaxation. Physical Review B, 2004, 70, .	3.2	11
212	Gold-Cage Perovskites: A Three-Dimensional Au^{III}â€“X Framework Encasing Isolated MX₆^{3â€“} Octahedra (M^{III} = In, Sb, Bi; X = Cl^{â€“},) Tj ETQq0 0 0 rgBT /Overlock 10 Tf	13.8	11
213	Ferroelectricity in [111]-oriented epitaxially strained <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:msub><mml:mi mathvariant="normal">SrTiO</mml:mi><mml:mn>3</mml:mn></mml:msub></mml:math> from first principles. Physical Review Materials, 2019, 3, .	2.4	11
214	Optimally tuned starting point for single-shot<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 of solids. Physical Review Materials, 2022, 6, .	2.4	11
215	Methane storage capabilities of diamond analogues. Physical Chemistry Chemical Physics, 2013, 15, 20937.	2.8	10
216	Emergence of topological electronic phases in elemental lithium under pressure. Proceedings of the National Academy of Sciences of the United States of America, 2019, 116, 9197-9201.	7.1	10

#	Article	IF	Citations
217	First-Principles Approach to the Conductance of Covalently Bound Molecular Junctions. Journal of Physical Chemistry C, 2019, 123, 6379-6387.	3.1	10
218	Band Edge Tailoring in Few-Layer Two-Dimensional Molybdenum Sulfide/Selenide Alloys. Journal of Physical Chemistry C, 2020, 124, 22893-22902.	3.1	9
219	Signatures of possible surface states in TaAs. Physical Review B, 2020, 102, .	3.2	9
220	Topological semimetal features in the multiferroic hexagonal manganites. Physical Review Materials, 2019, 3, .	2.4	9
221	The energy level alignment at metalâ€“molecule interfaces using Wannierâ€“Koopmans method. Applied Physics Letters, 2016, 108, .	3.3	8
222	Energy level alignment of self-assembled linear chains of benzenediamine on Au(111) from first principles. Physical Review B, 2016, 93, .	3.2	8
223	Theory and Simulation of Nanostructured Materials for Photovoltaic Applications. Computing in Science and Engineering, 2010, 12, 18-27.	1.2	7
224	Tuning the electronic structure of SrTiO3/SrFeO3â^'x superlattices via composition and vacancy control. APL Materials, 2014, 2, .	5.1	7
225	Superlattice-induced ferroelectricity in charge-ordered La _{1/3} Sr _{2/3} FeO ₃. Proceedings of the National Academy of Sciences of the United States of America, 2019, 116, 23972-23976.	7.1	7
226	Band Edge Energy Tuning through Electronic Character Hybridization in Ternary Metal Vanadates. Chemistry of Materials, 2021, 33, 7242-7253.	6.7	7
227	High Compressionâ€Induced Conductivity in a Layered Cuâ€“Br Perovskite. Angewandte Chemie, 2020, 132, 4046-4051.	2.0	7
228	Accelerated Discovery of CH₄ Uptake Capacity Metalâ€“Organic Frameworks Using Bayesian Optimization. Advanced Theory and Simulations, 2022, 5, .	2.8	7
229	An assessment of density functionals for predicting CO2 adsorption in diamine-functionalized metalâ€“organic frameworks. Journal of Chemical Physics, 2022, 156, 154113.	3.0	7
230	Algorithm for efficient elastic transport calculations for arbitrary device geometries. Physical Review B, 2011, 84, .	3.2	6
231	Push it to the limit: comparing periodic and local approaches to density functional theory for intermolecular interactions. Molecular Physics, 2019, 117, 1298-1305.	1.7	6
232	Expanded Analogs of Threeâ€Dimensional Leadâ€Halide Hybrid Perovskites. Angewandte Chemie, 2020, 132, 19249-19256.	2.0	6
233	Timeâ€Dependent Density Functional Theory of Narrow Band Gap Semiconductors Using a Screened Rangeâ€Separated Hybrid Functional. Advanced Theory and Simulations, 2020, 3, 2000220.	2.8	6
234	Addressing solar photochemistry durability with an amorphous nickel antimonate photoanode. Cell Reports Physical Science, 2022, 3, 100959.	5.6	6

#	Article	IF	Citations
235	From the interface energy to the solubility limit of aluminium in nickel from first-principles and Kinetic Monte Carlo calculations. Materials Science and Engineering B: Solid-State Materials for Advanced Technology, 2011, 176, 767-771.	3.5	5
236	First-principles studies of proton-Ba interactions in doped LaPO4. Journal of Materials Chemistry, 2012, 22, 3758.	6.7	5
237	Adsorption and Stability of Ï€-Bonded Ethylene on GaP(110). Journal of Physical Chemistry C, 2013, 117, 26091-26096.	3.1	5
238	Resonance Raman Characterization of Tetracene Monomer and Nanocrystals: Excited State Lattice Distortions With Implications For Efficient Singlet Fission. Journal of Physical Chemistry A, 2019, 123, 3863-3875.	2.5	5
239	Cooperative Carbon Dioxide Adsorption in Alcoholamineâ€•and Alkoxyalkylamineâ€Functionalized Metalâ€“Organic Frameworks. Angewandte Chemie, 2020, 132, 19636-19645.	2.0	5
240	Evolution of the Interfacial Electronic Structure During Thermal Oxidation. Springer Series in Materials Science, 2001, , 219-246.	0.6	5
241	Pressure amorphization through displacive disorder. European Physical Journal E, 2002, 9, 239-243.	1.6	4
242	Covalent Functionalization of GaP(110) Surfaces via a Staudinger-Type Reaction with Perfluorophenyl Azide. Journal of Physical Chemistry C, 2016, 120, 26448-26452.	3.1	4
243	Prediction of TiRhAs as a Dirac nodal line semimetal via first-principles calculations. Physical Review B, 2017, 96, .	3.2	4
244	Superexchange-induced valley splitting in two-dimensional transition metal dichalcogenides: A first-principles study for rational design. Physical Review B, 2021, 104, .	3.2	4
245	Elucidating heterogeneity in nanoplasmonic structures using nonlinear photon localization microscopy. Journal of Optics (United Kingdom), 2014, 16, 114014.	2.2	3
246	Dehydrogenation of Ammonia on Ru(0001) by Electronic Excitations. Journal of Physical Chemistry C, 2015, 119, 10520-10525.	3.1	3
247	Publisher's Note:Ab initiostudy of the phase diagram of epitaxialBaTiO3[Phys. Rev. B69, 212101 (2004)]. Physical Review B, 2004, 70, .	3.2	2
248	Interfacing carbon nanotubes of arbitrary chiralities into linear heterojunctions. Physical Review B, 2011, 83, .	3.2	2
249	Alkaline-stable nickel manganese oxides with ideal band gap for solar fuel photoanodes. Chemical Communications, 2018, 54, 4625-4628.	4.1	2
250	A diagrammatic approach for automatically deriving analytical gradients of tensor hyper-contracted electronic structure methods. Journal of Chemical Physics, 2021, 155, 024108.	3.0	2
251	Multidisciplinary Science at the Molecular Foundry. Advanced Materials, 2015, 27, 5634-5636.	21.0	1
252	Effective-Hamiltonian Modeling of External Pressures in Ferroelectric Perovskites. AIP Conference Proceedings, 2002, , .	0.4	0

#	Article	IF	Citations
253	Finite Time Domain Studies of Plasmonic Nano-structures Across Wide Frequency Ranges. , 2010, , .		0
254	Excitonic Properties of Lead-Halide Perovskites from First Principles Computational Modeling. , 0, , .		0
255	Excitonic Properties of Lead-Halide Perovskites from First Principles Computational Modeling. , 0, , .		0
256	Elucidation of Structural and Electronic Property Relationships in Hybrid Materials with High Pressure. , 0, , .		0