Jeffrey B Neaton

List of Publications by Year
in descending order

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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	Accelerated Discovery of CH₄ Uptake Capacity Metalâ€“Organic Frameworks Using Bayesian Optimization. Advanced Theory and Simulations, 2022, 5, .	2.8	7
2	Density of states prediction for materials discovery via contrastive learning from probabilistic embeddings. Nature Communications, 2022, 13, 949.	12.8	26
3	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
4	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
5	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><mml:mo stretchy="false">/</mml:mo><mml:mn>3</mml:mn><mml:mo>+</mml:mo><mml:mi>Î´</mml:mi></mml:mrow></mml:msub><mml:mn>1</mml:mn><mn Physical Review X, 2022, 12, .	8.9	14
6	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
7	Screening of Excitons by Organic Cations in Quasi-Two-Dimensional Organicâ€“Inorganic Lead-Halide Perovskites. Nano Letters, 2022, 22, 4870-4878.	9.1	24
8	Addressing solar photochemistry durability with an amorphous nickel antimonate photoanode. Cell Reports Physical Science, 2022, 3, 100959.	5.6	6
9	Anisotropic 2D excitons unveiled in organicâ€“inorganic quantum wells. Materials Horizons, 2021, 8, 197-208.	12.2	17
10	Reduced scaling formulation of CASPT2 analytical gradients using the supporting subspace method. Journal of Chemical Physics, 2021, 154, 014103.	3.0	19
11	Chemically Localized Resonant Excitons in Silverâ€“Pnictogen Halide Double Perovskites. Journal of Physical Chemistry Letters, 2021, 12, 2057-2063.	4.6	31
12	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	13.7	11
13	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>2</mml:mn><mml:mi>Mo</mml:mi><mml:mn>3</mml:mn><mml:mi>O</mml:mi><mml:mn>8</mml:mn></mml:mrow></mml:msub></mml:math> Physical Review B, 2021, 103, .	3.2	12
14	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
15	Exchange Bias in a Layered Metalâ€“Organic Topological Spin Glass. ACS Central Science, 2021, 7, 1317-1326.	11.3	17
16	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
17	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
18	Phonon Screening of Excitons in Semiconductors: Halide Perovskites and Beyond. Physical Review Letters, 2021, 127, 067401.	7.8	42

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19	Band Edge Energy Tuning through Electronic Character Hybridization in Ternary Metal Vanadates. Chemistry of Materials, 2021, 33, 7242-7253.	6.7	7
20	Directed assembly of layered perovskite heterostructures as single crystals. Nature, 2021, 597, 355-359.	27.8	58
21	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
22	High Compressionâ€Induced Conductivity in a Layered Cuâ€“Br Perovskite. Angewandte Chemie - International Edition, 2020, 59, 4017-4022.	13.8	23
23	Cooperative Carbon Dioxide Adsorption in Alcoholamineâ€•and Alkoxyalkylamineâ€Functionalized Metalâ€“Organic Frameworks. Angewandte Chemie - International Edition, 2020, 59, 19468-19477.	13.8	58
24	Band Edge Tailoring in Few-Layer Two-Dimensional Molybdenum Sulfide/Selenide Alloys. Journal of Physical Chemistry C, 2020, 124, 22893-22902.	3.1	9
25	Expanded Analogs of Threeâ€Dimensional Leadâ€Halide Hybrid Perovskites. Angewandte Chemie, 2020, 132, 19249-19256.	2.0	6
26	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
27	Cooperative carbon capture and steam regeneration with tetraamine-appended metalâ€“organic frameworks. Science, 2020, 369, 392-396.	12.6	249
28	Signatures of possible surface states in TaAs. Physical Review B, 2020, 102, .	3.2	9
29	Fermi-crossing Type-II Dirac fermions and topological surface states in NiTe2. Scientific Reports, 2020, 10, 12957.	3.3	29
30	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
31	Successes and Opportunities for Discovery of Metal Oxide Photoanodes for Solar Fuels Generators. ACS Energy Letters, 2020, 5, 1413-1421.	17.4	30
32	Band gap renormalization, carrier mobilities, and the electron-phonon self-energy in crystalline naphthalene. Physical Review B, 2020, 101, .	3.2	26
33	An automatically curated first-principles database of ferroelectrics. Scientific Data, 2020, 7, 72.	5.3	39
34	Expanded Analogs of Threeâ€Dimensional Leadâ€Halide Hybrid Perovskites. Angewandte Chemie - International Edition, 2020, 59, 19087-19094.	13.8	35
35	Cooperative Carbon Dioxide Adsorption in Alcoholamineâ€•and Alkoxyalkylamineâ€Functionalized Metalâ€“Organic Frameworks. Angewandte Chemie, 2020, 132, 19636-19645.	2.0	5
36	Carrier Diffusion Lengths Exceeding 1 Î¼m Despite Trap-Limited Transport in Halide Double Perovskites. ACS Energy Letters, 2020, 5, 1337-1345.	17.4	58

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37	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
38	Half-magnetization plateau and the origin of threefold symmetry breaking in an electrically switchable triangular antiferromagnet. Physical Review Research, 2020, 2, .	3.6	14
39	High Compressionâ€Induced Conductivity in a Layered Cuâ€“Br Perovskite. Angewandte Chemie, 2020, 132, 4046-4051.	2.0	7
40	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
41	Identifying substitutional oxygen as a prolific point defect in monolayer transition metal dichalcogenides. Nature Communications, 2019, 10, 3382.	12.8	196
42	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
43	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
44	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
45	First-Principles Approach to the Conductance of Covalently Bound Molecular Junctions. Journal of Physical Chemistry C, 2019, 123, 6379-6387.	3.1	10
46	Non-chemisorbed goldâ€“sulfur binding prevails in self-assembled monolayers. Nature Chemistry, 2019, 11, 351-358.	13.6	202
47	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
48	Tuning the bandgap of Cs₂AgBiBr₆ through dilute tin alloying. Chemical Science, 2019, 10, 10620-10628.	7.4	58
49	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
50	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
51	Topological semimetal features in the multiferroic hexagonal manganites. Physical Review Materials, 2019, 3, .	2.4	9
52	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
53	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></mml:m Physical Review Materials, 2019, 3, .	2.4	39
54	Detection of sub-MeV dark matter with three-dimensional Dirac materials. Physical Review D, 2018, 97, .	4.7	142

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55	Enrichment of molecular antenna triplets amplifies upconverting nanoparticle emission. Nature Photonics, 2018, 12, 402-407.	31.4	200
56	Alkaline-stable nickel manganese oxides with ideal band gap for solar fuel photoanodes. Chemical Communications, 2018, 54, 4625-4628.	4.1	2
57	Reducing Coercive-Field Scaling in Ferroelectric Thin Films via Orientation Control. ACS Nano, 2018, 12, 4736-4743.	14.6	47
58	Probing Charge Transport through Peptide Bonds. Journal of Physical Chemistry Letters, 2018, 9, 763-767.	4.6	38
59	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
60	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
61	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
62	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></mml:math> Physical Review B, 2018, 97, .	3.2	54
63	Layered Halide Double Perovskites: Dimensional Reduction of Cs₂AgBiBr₆. Journal of the American Chemical Society, 2018, 140, 5235-5240.	13.7	293
64	Topological materials discovery using electron filling constraints. Nature Physics, 2018, 14, 55-61.	16.7	39
65	Anisotropic Dirac Fermions in BaMnBi2 and BaZnBi2. Scientific Reports, 2018, 8, 15322.	3.3	14
66	Elucidating CO₂ Chemisorption in Diamine-Appended Metalâ€“Organic Frameworks. Journal of the American Chemical Society, 2018, 140, 18016-18031.	13.7	107
67	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
68	Defect-Induced Modification of Low-Lying Excitons and Valley Selectivity in Monolayer Transition Metal Dichalcogenides. Physical Review Letters, 2018, 121, 167402.	7.8	109
69	Formation of the layered conductive magnet CrCl2(pyrazine)2 through redox-active coordination chemistry. Nature Chemistry, 2018, 10, 1056-1061.	13.6	108
70	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
71	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
72	Cooperative Gas Adsorption without a Phase Transition in Metal-Organic Frameworks. Physical Review Letters, 2018, 121, 015701.	7.8	17

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73	Excited-state vibrational dynamics toward the polaron in methylammonium lead iodide perovskite. Nature Communications, 2018, 9, 2525.	12.8	129
74	Inversion symmetry and bulk Rashba effect in methylammonium lead iodide perovskite single crystals. Nature Communications, 2018, 9, 1829.	12.8	189
75	Smallâ€Bandâ€Gap Halide Double Perovskites. Angewandte Chemie, 2018, 130, 12947-12952.	2.0	19
76	Smallâ€Bandâ€Gap Halide Double Perovskites. Angewandte Chemie - International Edition, 2018, 57, 12765-12770.	13.8	136
77	Electron delocalization and charge mobility as a function of reduction in a metalâ€“organic framework. Nature Materials, 2018, 17, 625-632.	27.5	255
78	Energy level alignment at molecule-metal interfaces from an optimally tuned range-separated hybrid functional. Journal of Chemical Physics, 2017, 146, .	3.0	59
79	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
80	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
81	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
82	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
83	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
84	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
85	A reversible single-molecule switch based on activated antiaromaticity. Science Advances, 2017, 3, eaao2615.	10.3	94
86	Electronically Transparent Auâ€“N Bonds for Molecular Junctions. Journal of the American Chemical Society, 2017, 139, 14845-14848.	13.7	76
87	A direct look at halogen bonds. Science, 2017, 358, 167-168.	12.6	20
88	Voltage Dependence of Moleculeâ€“Electrode Coupling in Biased Molecular Junctions. Journal of Physical Chemistry C, 2017, 121, 21136-21144.	3.1	24
89	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
90	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

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91	Large Bulk Photovoltaic Effect and Spontaneous Polarization of Single-Layer Monochalcogenides. Physical Review Letters, 2017, 119, 067402.	7.8	182
92	Atomate: A high-level interface to generate, execute, and analyze computational materials science workflows. Computational Materials Science, 2017, 139, 140-152.	3.0	223
93	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
94	Origins of Singlet Fission in Solid Pentacene from an abÂinitio Greenâ€™s Function Approach. Physical Review Letters, 2017, 119, 267401.	7.8	55
95	Prediction of TiRhAs as a Dirac nodal line semimetal via first-principles calculations. Physical Review B, 2017, 96, .	3.2	4
96	The energy level alignment at metalâ€“molecule interfaces using Wannierâ€“Koopmans method. Applied Physics Letters, 2016, 108, .	3.3	8
97	First-principles Hubbard U approach for small molecule binding in metal-organic frameworks. Journal of Chemical Physics, 2016, 144, 174104.	3.0	73
98	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
99	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
100	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
101	Excited-State Properties of Molecular Solids from First Principles. Annual Review of Physical Chemistry, 2016, 67, 587-616.	10.8	88
102	Solar fuel photoanodes prepared by inkjet printing of copper vanadates. Journal of Materials Chemistry A, 2016, 4, 7483-7494.	10.3	56
103	Charge density wave order in 1D mirror twin boundaries of single-layer MoSe2. Nature Physics, 2016, 12, 751-756.	16.7	209
104	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
105	Electric Field- and Strain-Induced Rashba Effect in Hybrid Halide Perovskites. Journal of Physical Chemistry Letters, 2016, 7, 3683-3689.	4.6	104
106	Ab initioelectronic relaxation times and transport in noble metals. Physical Review B, 2016, 94, .	3.2	56
107	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><mml:mi>initiomany-body perturbation theory. Physical Review B, 2016, 94, .	3.2	14
108	Structural and excited-state properties of oligoacene crystals from first principles. Physical Review B, 2016, 93, .	3.2	89

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109	Ab initiophonon dispersion in crystalline naphthalene using van der Waals density functionals. Physical Review B, 2016, 93, .	3.2	41
110	molgw 1: Many-body perturbation theory software for atoms, molecules, and clusters. Computer Physics Communications, 2016, 208, 149-161.	7.5	139
111	Energy level alignment of self-assembled linear chains of benzenediamine on Au(111) from first principles. Physical Review B, 2016, 93, .	3.2	8
112	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
113	Mapping the Transmission Functions of Single-Molecule Junctions. Nano Letters, 2016, 16, 3949-3954.	9.1	58
114	Interplay of Bias-Driven Charging and the Vibrational Stark Effect in Molecular Junctions. Nano Letters, 2016, 16, 1104-1109.	9.1	40
115	Multidisciplinary Science at the Molecular Foundry. Advanced Materials, 2015, 27, 5634-5636.	21.0	1
116	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
117	Solid-state optical absorption from optimally tuned time-dependent range-separated hybrid density functional theory. Physical Review B, 2015, 92, .	3.2	210
118	Understanding Smallâ€Molecule Interactions in Metalâ€“Organic Frameworks: Coupling Experiment with Theory. Advanced Materials, 2015, 27, 5785-5796.	21.0	33
119	High Throughput Discovery of Solar Fuels Photoanodes in the CuOâ€“V₂O₅ System. Advanced Energy Materials, 2015, 5, 1500968.	19.5	82
120	Theory and computation of hot carriers generated by surface plasmon polaritons in noble metals. Nature Communications, 2015, 6, 7044.	12.8	317
121	Single-molecule diodes with high rectification ratios through environmental control. Nature Nanotechnology, 2015, 10, 522-527.	31.5	360
122	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
123	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
124	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
125	Mn₂V₂O₇: An Earth Abundant Light Absorber for Solar Water Splitting. Advanced Energy Materials, 2015, 5, 1401840.	19.5	61
126	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

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127	Cooperative insertion of CO2 in diamine-appended metal-organic frameworks. Nature, 2015, 519, 303-308.	27.8	1,026
128	Adsorption-Induced Solvent-Based Electrostatic Gating of Charge Transport through Molecular Junctions. Nano Letters, 2015, 15, 4498-4503.	9.1	34
129	CO₂ induced phase transitions in diamine-appended metalâ€“organic frameworks. Chemical Science, 2015, 6, 5177-5185.	7.4	45
130	Reliable Energy Level Alignment at Physisorbed Moleculeâ€“Metal Interfaces from Density Functional Theory. Nano Letters, 2015, 15, 2448-2455.	9.1	112
131	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
132	Dehydrogenation of Ammonia on Ru(0001) by Electronic Excitations. Journal of Physical Chemistry C, 2015, 119, 10520-10525.	3.1	3
133	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
134	GW100: Benchmarking G₀W₀ for Molecular Systems. Journal of Chemical Theory and Computation, 2015, 11, 5665-5687.	5.3	280
135	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
136	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
137	Relating the Physical Structure and Optoelectronic Function of Crystalline TIPSâ€Pentacene. Advanced Functional Materials, 2015, 25, 2038-2046.	14.9	77
138	Controlling the Thermoelectric Properties of Thiophene-Derived Single-Molecule Junctions. Chemistry of Materials, 2014, 26, 7229-7235.	6.7	52
139	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
140	Tuning the electronic structure of SrTiO3/SrFeO3â^'x superlattices via composition and vacancy control. APL Materials, 2014, 2, .	5.1	7
141	Ytterbium-driven strong enhancement of electron-phonon coupling in graphene. Physical Review B, 2014, 90, .	3.2	19
142	Elucidating heterogeneity in nanoplasmonic structures using nonlinear photon localization microscopy. Journal of Optics (United Kingdom), 2014, 16, 114014.	2.2	3
143	Tunable Charge Transport in Single-Molecule Junctions via Electrolytic Gating. Nano Letters, 2014, 14, 1400-1404.	9.1	107
144	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

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145	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
146	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
147	Thermoelectricity at the gate. Nature Nanotechnology, 2014, 9, 876-877.	31.5	16
148	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:m for closed-shell molecules. Physical Review B, 2014, 90, .	3.2	24
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