Emily Ann Carter

List of Publications by Year
in descending order

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435 papers	31,436 citations	3333 91 h-index	6643 156 g-index
458 all docs	458 docs citations	458 times ranked	23974 citing authors

#	Article	IF	Citations
1	Thermodynamic guiding principles of high-capacity phase transformation materials for splitting H₂O and CO₂ by thermochemical looping. Journal of Materials Chemistry A, 2022, 10, 3552-3561.	5.2	2
2	Reply to: Distinguishing thermal from non-thermal contributions to plasmonic hydrodefluorination. Nature Catalysis, 2022, 5, 247-250.	16.1	7
3	Identifying an Alternative Hydride Transfer Pathway for CO ₂ Reduction on CdTe(111) and CuInS ₂ (112) Surfaces. Advanced Theory and Simulations, 2022, 5, 2100413.	1.3	5
4	First-Principles Insights into Plasmon-Induced Catalysis. Annual Review of Physical Chemistry, 2021, 72, 99-119.	4.8	41
5	Precise Control of Nanoscale Cu Etching via Gas-Phase Oxidation and Chemical Complexation. Journal of Physical Chemistry C, 2021, 125, 1819-1832.	1.5	7
6	An Integrated Methodology for Screening Hydrogen Evolution Reaction Catalysts: Pt/Mo2C as an Example. Springer Series in Materials Science, 2021, , 719-731.	0.4	0
7	Optimizing kesterite solar cells from Cu₂ZnSnS₄ to Cu₂CdGe(S,Se)₄. Journal of Materials Chemistry A, 2021, 9, 9882-9897.	5.2	18
8	Autobiography of Emily A. Carter. Journal of Physical Chemistry C, 2021, 125, 4333-4341.	1.5	3
9	Autobiography of Emily A. Carter. Journal of Physical Chemistry A, 2021, 125, 1671-1679.	1.1	0
10	Revisiting Understanding of Electrochemical CO₂ Reduction on Cu(111): Competing Proton-Coupled Electron Transfer Reaction Mechanisms Revealed by Embedded Correlated Wavefunction Theory. Journal of the American Chemical Society, 2021, 143, 6152-6164.	6.6	65
11	Hot carrier multiplication in plasmonic photocatalysis. Proceedings of the National Academy of Sciences of the United States of America, 2021, 118, .	3.3	43
12	Metal-to-Ligand Charge-Transfer Spectrum of a Ru-Bipyridine-Sensitized TiO₂ Cluster from Embedded Multiconfigurational Excited-State Theory. Journal of Physical Chemistry A, 2021, 125, 4998-5013.	1.1	5
13	Projector-Free Capped-Fragment Scheme within Density Functional Embedding Theory for Covalent and Ionic Compounds. Journal of Chemical Theory and Computation, 2021, 17, 4105-4121.	2.3	3
14	Factors Governing Oxygen Vacancy Formation in Oxide Perovskites. Journal of the American Chemical Society, 2021, 143, 13212-13227.	6.6	75
15	Coupled Effects of Temperature, Pressure, and pH on Water Oxidation Thermodynamics and Kinetics. ACS Catalysis, 2021, 11, 11305-11319.	5.5	9
16	CO₂ Photoelectrochemical Reduction Catalyzed by a GaP(001) Photoelectrode. ACS Catalysis, 2021, 11, 1233-1241.	5.5	15
17	Assessing cathode property prediction via exchange-correlation functionals with and without long-range dispersion corrections. Physical Chemistry Chemical Physics, 2021, 23, 24726-24737.	1.3	8
18	Breaking a dative bond with mechanical forces. Nature Communications, 2021, 12, 5635.	5.8	17

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19	Relationship between ferroelectric polarization and stoichiometry of <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:msub><mml:mi>HfO</mml:mi><mml:mn>2</mml:mn></mml:msub></mml surfaces. Physical Review Materials, 2021, 5, .	3.1	4
20	Light-driven methane dry reforming with single atomic site antenna-reactor plasmonic photocatalysts. Nature Energy, 2020, 5, 61-70.	19.8	466
21	Deuterium addition to liquid Liâ€“Sn alloys: implications for plasma-facing applications. Nuclear Fusion, 2020, 60, 016025.	1.6	2
22	Benchmarking an Embedded Adaptive Sampling Configuration Interaction Method for Surface Reactions: H₂ Desorption from and CH₄ Dissociation on Cu(111). Journal of Chemical Theory and Computation, 2020, 16, 7078-7088.	2.3	23
23	Prediction of Highly Selective Electrocatalytic Nitrogen Reduction at Low Overpotential on a Mo-Doped g-GaN Monolayer. ACS Catalysis, 2020, 10, 12841-12857.	5.5	92
24	Microkinetic model for pH- and potential-dependent oxygen evolution during water splitting on Fe-doped Î²-NiOOH. Energy and Environmental Science, 2020, 13, 4962-4976.	15.6	46
25	Thermodynamics of Electrical Double Layers with Electrostatic Correlations. Journal of Physical Chemistry C, 2020, 124, 26830-26842.	1.5	10
26	First-Principles Modeling of Sodium Ion and Water Intercalation into Titanium Disulfide Interlayers for Water Desalination. Chemistry of Materials, 2020, 32, 10678-10687.	3.2	7
27	Exploring Caâ€“Ceâ€“Mâ€“O (M = 3d Transition Metal) Oxide Perovskites for Solar Thermochemical Applications. Chemistry of Materials, 2020, 32, 9964-9982.	3.2	49
28	Exchange-correlation functional challenges in modeling quaternary chalcogenides. Physical Review B, 2020, 102, .	1.1	15
29	Why Do We Use the Materials and Operating Conditions We Use for Heterogeneous (Photo)Electrochemical Water Splitting?. ACS Catalysis, 2020, 10, 11177-11234.	5.5	89
30	Discovering Competing Electrocatalytic Mechanisms and Their Overpotentials: Automated Enumeration of Oxygen Evolution Pathways. Journal of Physical Chemistry C, 2020, 124, 24883-24898.	1.5	7
31	Ionic Layering and Overcharging in Electrical Double Layers in a Poisson-Boltzmann Model. Physical Review Letters, 2020, 125, 188004.	2.9	28
32	Revisiting Competing Paths in Electrochemical CO₂ Reduction on Copper via Embedded Correlated Wavefunction Theory. Journal of Chemical Theory and Computation, 2020, 16, 6528-6538.	2.3	21
33	A Firstâ€Principlesâ€Based Subâ€Lattice Formalism for Predicting Offâ€Stoichiometry in Materials for Solar Thermochemical Applications: The Example of Ceria. Advanced Theory and Simulations, 2020, 3, 2000112.	1.3	10
34	Plasmon-driven carbonâ€“fluorine (C(sp3)â€“F) bond activation with mechanistic insights into hot-carrier-mediated pathways. Nature Catalysis, 2020, 3, 564-573.	16.1	81
35	Oxidation State of GaP Photoelectrode Surfaces under Electrochemical Conditions for Photocatalytic CO₂ Reduction. Journal of Physical Chemistry B, 2020, 124, 2255-2261.	1.2	3
36	Secondary Transition-Metal Dopants for Enhanced Electrochemical O2 Formation and Desorption on Fe-Doped Î²-NiOOH. ACS Energy Letters, 2020, 5, 962-967.	8.8	14

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37	Facet-Independent Oxygen Evolution Activity of Pure Î²-NiOOH: Different Chemistries Leading to Similar Overpotentials. Journal of the American Chemical Society, 2020, 142, 3600-3612.	6.6	114
38	Noninnocent Influence of Host Î²-NiOOH Redox Activity on Transition-Metal Dopantsâ€™ Efficacy as Active Sites in Electrocatalytic Water Oxidation. ACS Catalysis, 2020, 10, 2720-2734.	5.5	32
39	The generality of the GUGA MRCI approach in COLUMBUS for treating complex quantum chemistry. Journal of Chemical Physics, 2020, 152, 134110.	1.2	42
40	Evaluating optimal <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mi>U</mml:mi></mml:math> for <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mrow><mml:mn>3</mml:mn><mml:mi>d</mml:mi></mml:mrow></mml:r transition-metal oxides within the SCAN+ <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mi>U</mml:mi></mml:math> framework. Physical Review Materials, 2020, 4, .	0.9	55
41	Rationalizing the Hot-Carrier-Mediated Reaction Mechanisms and Kinetics for Ammonia Decomposition on Ruthenium-Doped Copper Nanoparticles. Journal of the American Chemical Society, 2019, 141, 13320-13323.	6.6	25
42	Surface-Plasmon-Induced Ammonia Decomposition on Copper: Excited-State Reaction Pathways Revealed by Embedded Correlated Wavefunction Theory. ACS Nano, 2019, 13, 9944-9957.	7.3	38
43	Upper bound to the gradient-based kinetic energy density of noninteracting electrons in an external potential. Journal of Chemical Physics, 2019, 151, 064113.	1.2	5
44	Suppressed Deep Traps and Bandgap Fluctuations in Cu₂CdSnS₄ Solar Cells with â‰ˆ8% Efficiency. Advanced Energy Materials, 2019, 9, 1902509.	10.2	65
45	Kinetic energy density of nearly free electrons. I. Response functionals of the external potential. Physical Review B, 2019, 100, .	1.1	11
46	Kinetic energy density of nearly free electrons. II. Response functionals of the electron density. Physical Review B, 2019, 100, .	1.1	12
47	Plasmonic Photocatalysis of Nitrous Oxide into N₂ and O₂ Using Aluminumâ€“Iridium Antennaâ€“Reactor Nanoparticles. ACS Nano, 2019, 13, 8076-8086.	7.3	83
48	Balancing Competing Reactions in Hydride Transfer Catalysis via Catalyst Surface Doping: The Ionization Energy Descriptor. Journal of the American Chemical Society, 2019, 141, 9895-9901.	6.6	9
49	Defect-Mediated Charge-Carrier Trapping and Nonradiative Recombination in WSe₂ Monolayers. Journal of the American Chemical Society, 2019, 141, 10451-10461.	6.6	81
50	Response to Comment on â€œQuantifying hot carrier and thermal contributions in plasmonic photocatalysisâ€. Science, 2019, 364, .	6.0	131
51	Plasmon damping depends on the chemical nature of the nanoparticle interface. Science Advances, 2019, 5, eaav0704.	4.7	128
52	Role of Na and Ca as Isovalent Dopants in Cu₂ZnSnS₄ Solar Cells. ACS Sustainable Chemistry and Engineering, 2019, 7, 5792-5800.	3.2	24
53	Properties of fusion-relevant liquid Li-Sn alloys: An ab initio molecular-dynamics study. Nuclear Materials and Energy, 2019, 18, 326-330.	0.6	2
54	Optimal functionalization of a molecular electrocatalyst for hydride transfer. Proceedings of the National Academy of Sciences of the United States of America, 2019, 116, 22953-22958.	3.3	4

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55	The technological and economic prospects for CO2 utilization and removal. Nature, 2019, 575, 87-97.	13.7	1,142
56	Subspace Density Matrix Functional Embedding Theory: Theory, Implementation, and Applications to Molecular Systems. Journal of Chemical Theory and Computation, 2019, 15, 949-960.	2.3	19
57	Theoretical Insights into Heterogeneous (Photo)electrochemical CO₂Reduction. Chemical Reviews, 2019, 119, 6631-6669.	23.0	431
58	Self-assembling of formic acid on the partially oxidizedp(2 Ã— 1) Cu(110) surface reconstruction at low coverages. Journal of Chemical Physics, 2019, 150, 041720.	1.2	3
59	Unraveling Oxygen Evolution on Iron-Doped Î²-Nickel Oxyhydroxide: The Key Role of Highly Active Molecular-like Sites. Journal of the American Chemical Society, 2019, 141, 693-705.	6.6	176
60	Hydride Shuttle Formation and Reaction with CO₂ on GaP(110). ChemSusChem, 2018, 11, 1558-1566.	3.6	19
61	Kohn-Sham potentials from electron densities using a matrix representation within finite atomic orbital basis sets. Journal of Chemical Physics, 2018, 148, 034105.	1.2	23
62	Kinetic and Mechanistic Effects of Bipyridine (bpy) Substituent, Labile Ligand, and BrÃ¸nsted Acid on Electrocatalytic CO₂ Reduction by Re(bpy) Complexes. ACS Catalysis, 2018, 8, 2021-2029.	5.5	155
63	Orbital-free density functional theory for materials research. Journal of Materials Research, 2018, 33, 777-795.	1.2	109
64	Mechanistic Insights into Photocatalyzed Hydrogen Desorption from Palladium Surfaces Assisted by Localized Surface Plasmon Resonances. ACS Nano, 2018, 12, 3512-3522.	7.3	62
65	Why and How Carbon Dioxide Conversion to Methanol Happens on Functionalized Semiconductor Photoelectrodes. Journal of the American Chemical Society, 2018, 140, 16749-16757.	6.6	16
66	Quantifying hot carrier and thermal contributions in plasmonic photocatalysis. Science, 2018, 362, 69-72.	6.0	756
67	Novel Solar Cell Materials: Insights from First-Principles. Journal of Physical Chemistry C, 2018, 122, 27107-27126.	1.5	20
68	Thermodynamic Evaluation of Trace-Amount Transition-Metal-Ion Doping in NiOOH Films. Journal of the Electrochemical Society, 2018, 165, F907-F913.	1.3	7
69	Potential Functional Embedding Theory with an Improved Kohnâ€“Sham Inversion Algorithm. Journal of Chemical Theory and Computation, 2018, 14, 5680-5689.	2.3	10
70	Orbital-free density functional theory simulation of collective dynamics coupling in liquid Sn. Journal of Chemical Physics, 2018, 149, 094504.	1.2	16
71	Dissociative Chemisorption of O₂ on Al(111): Dynamics on a Correlated Wave-Function-Based Potential Energy Surface. Journal of Physical Chemistry Letters, 2018, 9, 3271-3277.	2.1	40
72	Effect of transition-metal-ion dopants on the oxygen evolution reaction on NiOOH(0001). Physical Chemistry Chemical Physics, 2018, 20, 19525-19531.	1.3	33

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73	Effects of the Aqueous Environment on the Stability and Chemistry of Î²-NiOOH Surfaces. Chemistry of Materials, 2018, 30, 5205-5219.	3.2	41
74	Understanding the apparent fractional charge of protons in the aqueous electrochemical double layer. Nature Communications, 2018, 9, 3202.	5.8	47
75	2-Pyridinide as an Active Catalytic Intermediate for CO2 Reduction on p-GaP Photoelectrodes: Lifetime and Selectivity. Journal of the American Chemical Society, 2018, 140, 8732-8738.	6.6	19
76	Understanding the Effects of Cd and Ag Doping in Cu₂ZnSnS₄ Solar Cells. Chemistry of Materials, 2018, 30, 4543-4555.	3.2	76
77	Orbital-free density functional theory characterization of the <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mrow><mml:msup><mml:mi>I²</mml:mi><mml:mo>â€²</mml:mo></m mathvariant="normal">M</mml:mi><mml:msub><mml:mi mathvariant="normal">g</mml:mi><mml:mn>2</mml:mn></mml:msub><mml:mi mathvariant="normal">A</mml:mi><mml:msub><mml:mi mathvariant="normal">I</mml:mi><mml:mn>3</mml:mn></mml:msub></mml:mrow></mml:math>	0.9	3
78	Evaluating transition metal oxides within DFT-SCAN and <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mrow><mml:mtext>SCAN</mml:mtext><mml:mo>+</mml:mo><mml:mi> frameworks for solar thermochemical applications. Physical Review Materials, 2018, 2, .	0.9	37
79	Contributions to improving small ester combustion chemistry: Theory, model and experiments. Proceedings of the Combustion Institute, 2017, 36, 543-551.	2.4	42
80	Potential Functional Embedding Theory at the Correlated Wave Function Level. 1. Mixed Basis Set Embedding. Journal of Chemical Theory and Computation, 2017, 13, 1067-1080.	2.3	19
81	Potential Functional Embedding Theory at the Correlated Wave Function Level. 2. Error Sources and Performance Tests. Journal of Chemical Theory and Computation, 2017, 13, 1081-1093.	2.3	16
82	Structural and dynamic properties of liquid tin from a new modified embedded-atom method force field. Physical Review B, 2017, 95, .	1.1	22
83	Excited-State N₂ Dissociation Pathway on Fe-Functionalized Au. Journal of the American Chemical Society, 2017, 139, 4390-4398.	6.6	76
84	libKEDF: An accelerated library of kinetic energy density functionals. Journal of Computational Chemistry, 2017, 38, 1552-1559.	1.5	8
85	Local Electron Correlation Treatment in Extended Multireference Calculations: Effect of Acceptorâ€“Donor Substituents on the Biradical Character of the Polycyclic Aromatic Hydrocarbon Heptazethrene. Journal of Chemical Theory and Computation, 2017, 13, 2612-2622.	2.3	13
86	Theoretical Determination of Band Edge Alignments at the Waterâ€“CuInS₂(112) Semiconductor Interface. Langmuir, 2017, 33, 9479-9489.	1.6	6
87	Opinion: Quantum solutions for a sustainable energy future. Nature Reviews Chemistry, 2017, 1, .	13.8	18
88	The Holy Grail: Chemistry Enabling an Economically Viable CO₂ Capture, Utilization, and Storage Strategy. Accounts of Chemical Research, 2017, 50, 472-475.	7.6	153
89	The Role of Surface-Bound Dihydropyridine Analogues in Pyridine-Catalyzed CO₂ Reduction over Semiconductor Photoelectrodes. ACS Central Science, 2017, 3, 968-974.	5.3	22
90	Characterization of the liquid Li-solid Mo (1â€‰1â€‰0) interface from classical molecular dynamics for plasma-facing applications. Nuclear Fusion, 2017, 57, 116036.	1.6	7

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91	Hydride Transfer at the GaP(110)/Solution Interface: Mechanistic Implications for CO₂ Reduction Catalyzed by Pyridine. Journal of Physical Chemistry C, 2017, 121, 17321-17331.	1.5	18
92	Extending density functional embedding theory for covalently bonded systems. Proceedings of the National Academy of Sciences of the United States of America, 2017, 114, E10861-E10870.	3.3	21
93	Globally-Optimized Local Pseudopotentials for (Orbital-Free) Density Functional Theory Simulations of Liquids and Solids. Journal of Chemical Theory and Computation, 2017, 13, 3684-3695.	2.3	18
94	How To Identify Plasmons from the Optical Response of Nanostructures. ACS Nano, 2017, 11, 7321-7335.	7.3	72
95	A Density Functional +UAssessment of Oxygen Evolution Reaction Mechanisms on Î²-NiOOH. ACS Catalysis, 2017, 7, 5329-5339.	5.5	110
96	Prediction and characterization of an Mg-Al intermetallic compound with potentially improved ductility via orbital-free and Kohn-Sham density functional theory. Modelling and Simulation in Materials Science and Engineering, 2017, 25, 075002.	0.8	11
97	Prediction of a low-temperature N ₂ dissociation catalyst exploiting near-IRâ€“toâ€“visible light nanoplasmonics. Science Advances, 2017, 3, eaao4710.	4.7	74
98	Orbital-free density functional theory study of amorphous Liâ€“Si alloys and introduction of a simple density decomposition formalism. Modelling and Simulation in Materials Science and Engineering, 2016, 24, 035014.	0.8	4
99	Rock-salt structure lithium deuteride formation in liquid lithium with high-concentrations of deuterium: a first-principles molecular dynamics study. Nuclear Fusion, 2016, 56, 016020.	1.6	10
100	Cobalt (II) oxide and nickel (II) oxide alloys as potential intermediate-band semiconductors: A theoretical study. Journal of Applied Physics, 2016, 119, .	1.1	26
101	Density functional theory investigation of the electronic structure and defect chemistry of Sr1-xKxFeO3. MRS Communications, 2016, 6, 145-150.	0.8	3
102	Effect of Temperature on the Desorption of Lithium from Molybdenum(110) Surfaces: Implications for Fusion Reactor First Wall Materials. Journal of Physical Chemistry B, 2016, 120, 6110-6119.	1.2	15
103	Density functional theory + U analysis of the electronic structure and defect chemistry of LSCF (La_{0.5}Sr_{0.5}Co_{0.25}Fe_{0.75}O_{3â^'Î´}). Physical Chemistry Chemical Physics, 2016, 18, 12260-12269.	1.3	39
104	Petascale Orbital-Free Density Functional Theory Enabled by Small-Box Algorithms. Journal of Chemical Theory and Computation, 2016, 12, 2950-2963.	2.3	41
105	Understanding and Tuning the Hydrogen Evolution Reaction on Pt-Covered Tungsten Carbide Cathodes. Journal of the Electrochemical Society, 2016, 163, F629-F636.	1.3	15
106	Stability of surface protons in pyridine-catalyzed CO₂ reduction at p-GaP photoelectrodes. Physical Chemistry Chemical Physics, 2016, 18, 26434-26443.	1.3	21
107	Surface Energy as a Descriptor of Catalytic Activity. Journal of Physical Chemistry C, 2016, 120, 23698-23706.	1.5	83
108	Is the Surface Playing a Role during Pyridine-Catalyzed CO₂ Reduction on p-GaP Photoelectrodes?. ACS Energy Letters, 2016, 1, 464-468.	8.8	34

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109	Interaction of Pyridine and Water with the Reconstructed Surfaces of GaP(111) and CdTe(111) Photoelectrodes: Implications for CO2 Reduction. Chemistry of Materials, 2016, 28, 5799-5810.	3.2	42
110	Heterometallic antennaâ^'reactor complexes for photocatalysis. Proceedings of the National Academy of Sciences of the United States of America, 2016, 113, 8916-8920.	3.3	381
111	Elastic and Thermodynamic Properties of Complex Mg-Al Intermetallic Compounds via Orbital-Free Density Functional Theory. Physical Review Applied, 2016, 5, .	1.5	30
112	Determining and Controlling the Stoichiometry of Cu₂ZnSnS₄ Photovoltaics: The Physics and Its Implications. Chemistry of Materials, 2016, 28, 4415-4420.	3.2	28
113	Spin-Free [2]_{R12} Basis Set Incompleteness Correction to the Local Multireference Configuration Interaction and the Local Multireference Average Coupled Pair Functional Methods. Journal of Chemical Theory and Computation, 2016, 12, 3176-3184.	2.3	3
114	Elucidating Structural Disorder and the Effects of Cu Vacancies on the Electronic Properties of Cu₂ZnSnS₄. Chemistry of Materials, 2016, 28, 864-869.	3.2	36
115	Ab initio kinetics studies of hydrogen atom abstraction from methyl propanoate. Physical Chemistry Chemical Physics, 2016, 18, 4594-4607.	1.3	35
116	Aluminum Nanocrystals as a Plasmonic Photocatalyst for Hydrogen Dissociation. Nano Letters, 2016, 16, 1478-1484.	4.5	294
117	Corrigendum to: Plasmon-Driven Dissociation of H₂ on Gold Nanoclusters. Zeitschrift Fur Physikalische Chemie, 2016, 230, 131-132.	1.4	8
118	Thermodynamic Constraints in Using AuM (M = Fe, Co, Ni, and Mo) Alloys as N₂ Dissociation Catalysts: Functionalizing a Plasmon-Active Metal. ACS Nano, 2016, 10, 2940-2949.	7.3	40
119	Ab Initio Reaction Kinetics of CH₃OÄŠ(â•Ö) and ÄŠH₂OC(â•Ö)H Radicals. Journal of Physical Chemistry B, 2016, 120, 1590-1600.	1.2	43
120	Reply to â€œComment on â€˜Single-point kinetic energy density functionals: A pointwise kinetic energy density analysis and numerical convergence investigationâ€™â€‰â€•. Physical Review B, 2015, 92, .	1.1	14
121	Implementation of density functional embedding theory within the projector-augmented-wave method and applications to semiconductor defect states. Journal of Chemical Physics, 2015, 143, 102806.	1.2	46
122	Three-dimensional hole transport in nickel oxide by alloying with MgO or ZnO. Journal of Applied Physics, 2015, 118, 185102.	1.1	7
123	Orbital-Resolved Imaging of the Adsorbed State of Pyridine on GaP(110) Identifies Sites Susceptible to Nucleophilic Attack. Journal of Physical Chemistry C, 2015, 119, 28917-28924.	1.5	8
124	Liquid li structure and dynamics: A comparison between OFDFT and second nearestâ€neighbor embeddedâ€atom method. AICHE Journal, 2015, 61, 2841-2853.	1.8	24
125	Ab Initio Kinetics of Hydrogen Abstraction from Methyl Acetate by Hydrogen, Methyl, Oxygen, Hydroxyl, and Hydroperoxy Radicals. Journal of Physical Chemistry A, 2015, 119, 6377-6390.	1.1	43
126	Strategies to suppress cation vacancies in metal oxide alloys: consequences for solar energy conversion. Journal of Materials Science, 2015, 50, 5715-5722.	1.7	8

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127	Single-point kinetic energy density functionals: A pointwise kinetic energy density analysis and numerical convergence investigation. Physical Review B, 2015, 91, .	1.1	46
128	Cluster Models for Studying CO2 Reduction on Semiconductor Photoelectrodes. Topics in Catalysis, 2015, 58, 46-56.	1.3	30
129	Observation of Surface-Bound Negatively Charged Hydride and Hydroxide on GaP(110) in H₂O Environments. Journal of Physical Chemistry C, 2015, 119, 17762-17772.	1.5	39
130	First-principles assessment of hole transport in pure and Li-doped NiO. Physical Chemistry Chemical Physics, 2015, 17, 18098-18110.	1.3	22
131	Dissociative Adsorption of O₂ on Al(111): The Role of Orientational Degrees of Freedom. Journal of Physical Chemistry Letters, 2015, 6, 1661-1665.	2.1	41
132	Cooperative Effects in Water Binding to Cuprous Oxide Surfaces. Journal of Physical Chemistry C, 2015, 119, 9311-9323.	1.5	38
133	Introducing PROFESS 3.0: An advanced program for orbital-free density functional theory molecular dynamics simulations. Computer Physics Communications, 2015, 190, 228-230.	3.0	67
134	Bond Dissociation Energies of C₁₀ and C₁₈ Methyl Esters from Local Multireference Averaged-Coupled Pair Functional Theory. Journal of Physical Chemistry A, 2015, 119, 3429-3439.	1.1	27
135	A Strategy to Stabilize Kesterite CZTS for High-Performance Solar Cells. Chemistry of Materials, 2015, 27, 2920-2927.	3.2	63
136	What Is the Role of Pyridinium in Pyridine-Catalyzed CO₂ Reduction on p-GaP Photocathodes?. Journal of the American Chemical Society, 2015, 137, 13248-13251.	6.6	63
137	Ab initio pressure-dependent reaction kinetics of methyl propanoate radicals. Physical Chemistry Chemical Physics, 2015, 17, 31061-31072.	1.3	17
138	Density Fitting and Cholesky Decomposition of the Two-Electron Integrals in Local Multireference Configuration Interaction Theory. Journal of Chemical Theory and Computation, 2015, 11, 5242-5251.	2.3	14
139	Structural and Electronic Features of Î²-Ni(OH)₂ and Î²-NiOOH from First Principles. Journal of Physical Chemistry C, 2015, 119, 24315-24322.	1.5	145
140	Ab Initio Unimolecular Reaction Kinetics of CH2C(â•Ö)OCH3 and CH3C(â•Ö)OCH2 Radicals. Journal of Physical Chemistry A, 2015, 119, 10553-10562.	1.1	16
141	Influence of Weak BrÃ¸nsted Acids on Electrocatalytic CO₂ Reduction by Manganese and Rhenium Bipyridine Catalysts. ACS Catalysis, 2015, 5, 900-908.	5.5	120
142	Assessment of a semi integral-direct local multi-reference configuration interaction implementation employing shared-memory parallelization. Computational and Theoretical Chemistry, 2015, 1051, 47-56.	1.1	9
143	Kinetic studies of methyl acetate pyrolysis and oxidation in a flow reactor and a low-pressure flat flame using molecular-beam mass spectrometry. Proceedings of the Combustion Institute, 2015, 35, 491-498.	2.4	45
144	Shared-memory parallelization of a local correlation multi-reference CI program. Computer Physics Communications, 2014, 185, 3175-3188.	3.0	8

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145	Firstâ€Principles Modeling of Electrochemical Water Oxidation on MnO:ZnO(001). ChemElectroChem, 2014, 1, 407-415.	1.7	19
146	Communication: Comparing ab initio methods of obtaining effective U parameters for closed-shell materials. Journal of Chemical Physics, 2014, 140, 121105.	1.2	61
147	Significant Reduction in NiO Band Gap Upon Formation of Li_xNi_{1â^'x}O alloys: Applications To Solar Energy Conversion. ChemSusChem, 2014, 7, 195-201.	3.6	56
148	Time-dependent potential-functional embedding theory. Journal of Chemical Physics, 2014, 140, 124113.	1.2	22
149	Size-extensivity-corrected multireference configuration interaction schemes to accurately predict bond dissociation energies of oxygenated hydrocarbons. Journal of Chemical Physics, 2014, 140, 044317.	1.2	85
150	Analysis of and remedies for unphysical ground states of the multireference averaged coupled-pair functional. Journal of Chemical Physics, 2014, 140, 024102.	1.2	6
151	First-principles simulations of plasticity in body-centered-cubic magnesiumâ€“lithium alloys. Acta Materialia, 2014, 64, 198-207.	3.8	41
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