Emily Ann Carter

List of Publications by Year in Descending Order

430 papers	25,127 citations	85 h-index	138 g-index
458 ext. papers	28,157 ext. citations	7.1 avg, IF	7.69 L-index

#	Paper	IF	Citations
430	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	3.5	0
429	Assessing cathode property prediction exchange-correlation functionals with and without long-range dispersion corrections. *Physical Chemistry Chemical Physics*, **2021**, 23, 24726-24737	3.6	2
428	Breaking a dative bond with mechanical forces. *Nature Communications*, **2021**, 12, 5635	17.4	9
427	Revisiting Understanding of Electrochemical CO 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	16.4	18
426	Hot carrier multiplication in plasmonic photocatalysis. *Proceedings of the National Academy of Sciences of the United States of America*, **2021**, 118,	11.5	12
425	Metal-to-Ligand Charge-Transfer Spectrum of a Ru-Bipyridine-Sensitized TiO Cluster from Embedded Multiconfigurational Excited-State Theory. *Journal of Physical Chemistry A*, **2021**, 125, 4998-5013	2.8	1
424	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	6.4	1
423	First-Principles Insights into Plasmon-Induced Catalysis. *Annual Review of Physical Chemistry*, **2021**, 72, 99-119	15.7	14
422	Precise Control of Nanoscale Cu Etching via Gas-Phase Oxidation and Chemical Complexation. *Journal of Physical Chemistry C*, **2021**, 125, 1819-1832	3.8	3
421	An Integrated Methodology for Screening Hydrogen Evolution Reaction Catalysts: Pt/Mo2C as an Example. *Springer Series in Materials Science*, **2021**, 719-731	0.9	
420	Optimizing kesterite solar cells from Cu2ZnSnS4 to Cu2CdGe(S,Se)4. *Journal of Materials Chemistry A*, **2021**, 9, 9882-9897	13	5
419	Factors Governing Oxygen Vacancy Formation in Oxide Perovskites. *Journal of the American Chemical Society*, **2021**, 143, 13212-13227	16.4	10
418	Coupled Effects of Temperature, Pressure, and pH on Water Oxidation Thermodynamics and Kinetics. *ACS Catalysis*, **2021**, 11, 11305-11319	13.1	3
417	CO2 Photoelectrochemical Reduction Catalyzed by a GaP(001) Photoelectrode. *ACS Catalysis*, **2021**, 11, 1233-1241	13.1	3
416	Plasmon-driven carbon□luorine (C(sp3)□) bond activation with mechanistic insights into hot-carrier-mediated pathways. *Nature Catalysis*, **2020**, 3, 564-573	36.5	29
415	Oxidation State of GaP Photoelectrode Surfaces under Electrochemical Conditions for Photocatalytic CO Reduction. *Journal of Physical Chemistry B*, **2020**, 124, 2255-2261	3.4	2
414	Secondary Transition-Metal Dopants for Enhanced Electrochemical O2 Formation and Desorption on Fe-Doped □NiOOH. *ACS Energy Letters*, **2020**, 5, 962-967	20.1	10

413	Facet-Independent Oxygen Evolution Activity of Pure β-NiOOH: Different Chemistries Leading to Similar Overpotentials. *Journal of the American Chemical Society*, **2020**, 142, 3600-3612	16.4	61
412	Noninnocent Influence of Host β-NiOOH Redox Activity on Transition-Metal Dopants' Efficacy as Active Sites in Electrocatalytic Water Oxidation. *ACS Catalysis*, **2020**, 10, 2720-2734	13.1	16
411	The generality of the GUGA MRCI approach in COLUMBUS for treating complex quantum chemistry. *Journal of Chemical Physics*, **2020**, 152, 134110	3.9	22
410	Evaluating optimal U for 3d transition-metal oxides within the SCAN+U framework. *Physical Review Materials*, **2020**, 4,	3.2	21
409	Light-driven methane dry reforming with single atomic site antenna-reactor plasmonic photocatalysts. *Nature Energy*, **2020**, 5, 61-70	62.3	213
408	Deuterium addition to liquid Li-Sn alloys: implications for plasma-facing applications. *Nuclear Fusion*, **2020**, 60, 016025	3.3	1
407	Benchmarking an Embedded Adaptive Sampling Configuration Interaction Method for Surface Reactions: H Desorption from and CH Dissociation on Cu(111). *Journal of Chemical Theory and Computation*, **2020**, 16, 7078-7088	6.4	11
406	Prediction of Highly Selective Electrocatalytic Nitrogen Reduction at Low Overpotential on a Mo-Doped g-GaN Monolayer. *ACS Catalysis*, **2020**, 10, 12841-12857	13.1	37
405	Microkinetic model for pH- and potential-dependent oxygen evolution during water splitting on Fe-doped β-NiOOH. *Energy and Environmental Science*, **2020**, 13, 4962-4976	35.4	23
404	Thermodynamics of Electrical Double Layers with Electrostatic Correlations. *Journal of Physical Chemistry C*, **2020**, 124, 26830-26842	3.8	2
403	First-Principles Modeling of Sodium Ion and Water Intercalation into Titanium Disulfide Interlayers for Water Desalination. *Chemistry of Materials*, **2020**, 32, 10678-10687	9.6	3
402	Exploring $Ca_{1-x}M_xO_{3-\delta}$ (M = 3d Transition Metal) Oxide Perovskites for Solar Thermochemical Applications. *Chemistry of Materials*, **2020**, 32, 9964-9982	9.6	11
401	Exchange-correlation functional challenges in modeling quaternary chalcogenides. *Physical Review B*, **2020**, 102,	3.3	7
400	Why Do We Use the Materials and Operating Conditions We Use for Heterogeneous (Photo)Electrochemical Water Splitting?. *ACS Catalysis*, **2020**, 10, 11177-11234	13.1	36
399	Discovering Competing Electrocatalytic Mechanisms and Their Overpotentials: Automated Enumeration of Oxygen Evolution Pathways. *Journal of Physical Chemistry C*, **2020**, 124, 24883-24898	3.8	5
398	Ionic Layering and Overcharging in Electrical Double Layers in a Poisson-Boltzmann Model. *Physical Review Letters*, **2020**, 125, 188004	7.4	8
397	Revisiting Competing Paths in Electrochemical CO Reduction on Copper via Embedded Correlated Wavefunction Theory. *Journal of Chemical Theory and Computation*, **2020**, 16, 6528-6538	6.4	10
396	A First-Principles-Based Sub-Lattice Formalism for Predicting Off-Stoichiometry in Materials for Solar Thermochemical Applications: The Example of Ceria. *Advanced Theory and Simulations*, **2020**, 3, 2000112	3.5	4

395	Kinetic energy density of nearly free electrons. I. Response functionals of the external potential. *Physical Review B*, **2019**, 100,	3.3	4
394	Kinetic energy density of nearly free electrons. II. Response functionals of the electron density. *Physical Review B*, **2019**, 100,	3.3	7
393	Plasmonic Photocatalysis of Nitrous Oxide into N and O Using Aluminum-Iridium Antenna-Reactor Nanoparticles. *ACS Nano*, **2019**, 13, 8076-8086	16.7	55
392	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	16.4	7
391	Defect-Mediated Charge-Carrier Trapping and Nonradiative Recombination in WSe Monolayers. *Journal of the American Chemical Society*, **2019**, 141, 10451-10461	16.4	48
390	Response to Comment on "Quantifying hot carrier and thermal contributions in plasmonic photocatalysis". *Science*, **2019**, 364,	33.3	102
389	Plasmon damping depends on the chemical nature of the nanoparticle interface. *Science Advances*, **2019**, 5, eaav0704	14.3	80
388	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	16.4	15
387	Surface-Plasmon-Induced Ammonia Decomposition on Copper: Excited-State Reaction Pathways Revealed by Embedded Correlated Wavefunction Theory. *ACS Nano*, **2019**, 13, 9944-9957	16.7	26
386	Upper bound to the gradient-based kinetic energy density of noninteracting electrons in an external potential. *Journal of Chemical Physics*, **2019**, 151, 064113	3.9	2
385	Suppressed Deep Traps and Bandgap Fluctuations in Cu2CdSnS4 Solar Cells with 8% Efficiency. *Advanced Energy Materials*, **2019**, 9, 1902509	21.8	37
384	Role of Na and Ca as Isovalent Dopants in Cu2ZnSnS4 Solar Cells. *ACS Sustainable Chemistry and Engineering*, **2019**, 7, 5792-5800	8.3	15
383	Properties of fusion-relevant liquid Li-Sn alloys: An ab initio molecular-dynamics study. *Nuclear Materials and Energy*, **2019**, 18, 326-330	2.1	2
382	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	11.5	3
381	The technological and economic prospects for CO utilization and removal. *Nature*, **2019**, 575, 87-97	50.4	479
380	Subspace Density Matrix Functional Embedding Theory: Theory, Implementation, and Applications to Molecular Systems. *Journal of Chemical Theory and Computation*, **2019**, 15, 949-960	6.4	15
379	Theoretical Insights into Heterogeneous (Photo)electrochemical CO Reduction. *Chemical Reviews*, **2019**, 119, 6631-6669	68.1	238
378	Self-assembling of formic acid on the partially oxidized p(2 1) Cu(110) surface reconstruction at low coverages. *Journal of Chemical Physics*, **2019**, 150, 041720	3.9	3

377	Unraveling Oxygen Evolution on Iron-Doped Nickel Oxyhydroxide: The Key Role of Highly Active Molecular-like Sites. *Journal of the American Chemical Society*, **2019**, 141, 693-705	16.4	108
376	Hydride Shuttle Formation and Reaction with CO on GaP(110). *ChemSusChem*, **2018**, 11, 1558-1566	8.3	13
375	Kohn-Sham potentials from electron densities using a matrix representation within finite atomic orbital basis sets. *Journal of Chemical Physics*, **2018**, 148, 034105	3.9	16
374	Kinetic and Mechanistic Effects of Bipyridine (bpy) Substituent, Labile Ligand, and Brønsted Acid on Electrocatalytic CO2 Reduction by Re(bpy) Complexes. *ACS Catalysis*, **2018**, 8, 2021-2029	13.1	117
373	Orbital-free density functional theory for materials research. *Journal of Materials Research*, **2018**, 33, 777-795	2.5	68
372	Mechanistic Insights into Photocatalyzed Hydrogen Desorption from Palladium Surfaces Assisted by Localized Surface Plasmon Resonances. *ACS Nano*, **2018**, 12, 3512-3522	16.7	46
371	Effects of the Aqueous Environment on the Stability and Chemistry of NiOOH Surfaces. *Chemistry of Materials*, **2018**, 30, 5205-5219	9.6	25
370	Understanding the apparent fractional charge of protons in the aqueous electrochemical double layer. *Nature Communications*, **2018**, 9, 3202	17.4	31
369	2-Pyridinide as an Active Catalytic Intermediate for CO Reduction on p-GaP Photoelectrodes: Lifetime and Selectivity. *Journal of the American Chemical Society*, **2018**, 140, 8732-8738	16.4	13
368	Understanding the Effects of Cd and Ag Doping in Cu2ZnSnS4 Solar Cells. *Chemistry of Materials*, **2018**, 30, 4543-4555	9.6	54
367	Orbital-free density functional theory characterization of the Mg2Al3 Samson phase. *Physical Review Materials*, **2018**, 2,	3.2	2
366	Evaluating transition metal oxides within DFT-SCAN and SCAN+U frameworks for solar thermochemical applications. *Physical Review Materials*, **2018**, 2,	3.2	50
365	Why and How Carbon Dioxide Conversion to Methanol Happens on Functionalized Semiconductor Photoelectrodes. *Journal of the American Chemical Society*, **2018**, 140, 16749-16757	16.4	10
364	Quantifying hot carrier and thermal contributions in plasmonic photocatalysis. *Science*, **2018**, 362, 69-72	33.3	494
363	Novel Solar Cell Materials: Insights from First-Principles. *Journal of Physical Chemistry C*, **2018**, 122, 27107-27126	3.8	69
362	Thermodynamic Evaluation of Trace-Amount Transition-Metal-Ion Doping in NiOOH Films. *Journal of the Electrochemical Society*, **2018**, 165, F907-F913	3.9	5
361	Potential Functional Embedding Theory with an Improved Kohn-Sham Inversion Algorithm. *Journal of Chemical Theory and Computation*, **2018**, 14, 5680-5689	6.4	5
360	Orbital-free density functional theory simulation of collective dynamics coupling in liquid Sn. *Journal of Chemical Physics*, **2018**, 149, 094504	3.9	12

359	Dissociative Chemisorption of O on Al(111): Dynamics on a Correlated Wave-Function-Based Potential Energy Surface. *Journal of Physical Chemistry Letters*, **2018**, 9, 3271-3277	6.4	28
358	Effect of transition-metal-ion dopants on the oxygen evolution reaction on NiOOH(0001). *Physical Chemistry Chemical Physics*, **2018**, 20, 19525-19531	3.6	22
357	Contributions to improving small ester combustion chemistry: Theory, model and experiments. *Proceedings of the Combustion Institute*, **2017**, 36, 543-551	5.9	38
356	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	6.4	14
355	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	6.4	12
354	Structural and dynamic properties of liquid tin from a new modified embedded-atom method force field. *Physical Review B*, **2017**, 95,	3.3	12
353	Excited-State N Dissociation Pathway on Fe-Functionalized Au. *Journal of the American Chemical Society*, **2017**, 139, 4390-4398	16.4	61
352	Local Electron Correlation Treatment in Extended Multireference Calculations: Effect of Acceptor-Donor Substituents on the Biradical Character of the Polycyclic Aromatic Hydrocarbon Heptazethrene. *Journal of Chemical Theory and Computation*, **2017**, 13, 2612-2622	6.4	10
351	Theoretical Determination of Band Edge Alignments at the Water-CuInS(112) Semiconductor Interface. *Langmuir*, **2017**, 33, 9479-9489	4	5
350	Opinion: Quantum solutions for a sustainable energy future. *Nature Reviews Chemistry*, **2017**, 1,	34.6	12
349	The Holy Grail: Chemistry Enabling an Economically Viable CO Capture, Utilization, and Storage Strategy. *Accounts of Chemical Research*, **2017**, 50, 472-475	24.3	114
348	Density and Potential Functional Embedding: Theory and Practice **2017**, 81-117		20
347	The Role of Surface-Bound Dihydropyridine Analogues in Pyridine-Catalyzed CO Reduction over Semiconductor Photoelectrodes. *ACS Central Science*, **2017**, 3, 968-974	16.8	21
346	Characterization of the liquid Li-solid Mo (1 1 0) interface from classical molecular dynamics for plasma-facing applications. *Nuclear Fusion*, **2017**, 57, 116036	3.3	4
345	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	3.8	15
344	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	11.5	17
343	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	6.4	13
342	How To Identify Plasmons from the Optical Response of Nanostructures. *ACS Nano*, **2017**, 11, 7321-7335	16.7	54

341	A Density Functional + U Assessment of Oxygen Evolution Reaction Mechanisms on □NiOOH. *ACS Catalysis*, **2017**, 7, 5329-5339	13.1	82
340	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	2	7
339	Prediction of a low-temperature N dissociation catalyst exploiting near-IR-to-visible light nanoplasmonics. *Science Advances*, **2017**, 3, eaao4710	14.3	57
338	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	9.6	37
337	Heterometallic antenna-reactor complexes for photocatalysis. *Proceedings of the National Academy of Sciences of the United States of America*, **2016**, 113, 8916-20	11.5	272
336	Elastic and Thermodynamic Properties of Complex Mg-Al Intermetallic Compounds via Orbital-Free Density Functional Theory. *Physical Review Applied*, **2016**, 5,	4.3	20
335	Determining and Controlling the Stoichiometry of Cu2ZnSnS4 Photovoltaics: The Physics and Its Implications. *Chemistry of Materials*, **2016**, 28, 4415-4420	9.6	24
334	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, 3176-84	6.4	2
333	Elucidating Structural Disorder and the Effects of Cu Vacancies on the Electronic Properties of Cu2ZnSnS4. *Chemistry of Materials*, **2016**, 28, 864-869	9.6	30
332	Ab initio kinetics studies of hydrogen atom abstraction from methyl propanoate. *Physical Chemistry Chemical Physics*, **2016**, 18, 4594-607	3.6	29
331	Aluminum Nanocrystals as a Plasmonic Photocatalyst for Hydrogen Dissociation. *Nano Letters*, **2016**, 16, 1478-84	11.5	234
330	Corrigendum to: Plasmon-Driven Dissociation of H2 on Gold Nanoclusters. *Zeitschrift Fur Physikalische Chemie*, **2016**, 230, 131-132	3.1	8
329	Thermodynamic Constraints in Using AuM (M = Fe, Co, Ni, and Mo) Alloys as N□Dissociation Catalysts: Functionalizing a Plasmon-Active Metal. *ACS Nano*, **2016**, 10, 2940-9	16.7	34
328	Ab Initio Reaction Kinetics of CH3O(?O) and □H2OC(?O)H Radicals. *Journal of Physical Chemistry B*, **2016**, 120, 1590-600	3.4	32
327	Orbital-free density functional theory study of amorphous Li□Si alloys and introduction of a simple density decomposition formalism. *Modelling and Simulation in Materials Science and Engineering*, **2016**, 24, 035014	2	3
326	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	3.3	10
325	Cobalt (II) oxide and nickel (II) oxide alloys as potential intermediate-band semiconductors: A theoretical study. *Journal of Applied Physics*, **2016**, 119, 025102	2.5	15
324	Density functional theory investigation of the electronic structure and defect chemistry of Sr1-xKxFeO3. *MRS Communications*, **2016**, 6, 145-150	2.7	3

323	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, 6110-9	3.4	12
322	Density functional theory + U analysis of the electronic structure and defect chemistry of LSCF (La0.5Sr0.5Co0.25Fe0.75O3-δ). *Physical Chemistry Chemical Physics*, **2016**, 18, 12260-9	3.6	31
321	Petascale Orbital-Free Density Functional Theory Enabled by Small-Box Algorithms. *Journal of Chemical Theory and Computation*, **2016**, 12, 2950-63	6.4	25
320	Understanding and Tuning the Hydrogen Evolution Reaction on Pt-Covered Tungsten Carbide Cathodes. *Journal of the Electrochemical Society*, **2016**, 163, F629-F636	3.9	13
319	Stability of surface protons in pyridine-catalyzed CO reduction at p-GaP photoelectrodes. *Physical Chemistry Chemical Physics*, **2016**, 18, 26434-26443	3.6	19
318	Surface Energy as a Descriptor of Catalytic Activity. *Journal of Physical Chemistry C*, **2016**, 120, 23698-23706	3.8	60
317	Is the Surface Playing a Role during Pyridine-Catalyzed CO2 Reduction on p-GaP Photoelectrodes?. *ACS Energy Letters*, **2016**, 1, 464-468	20.1	31
316	Observation of Surface-Bound Negatively Charged Hydride and Hydroxide on GaP(110) in H2O Environments. *Journal of Physical Chemistry C*, **2015**, 119, 17762-17772	3.8	35
315	First-principles assessment of hole transport in pure and Li-doped NiO. *Physical Chemistry Chemical Physics*, **2015**, 17, 18098-110	3.6	17
314	Dissociative Adsorption of O2 on Al(111): The Role of Orientational Degrees of Freedom. *Journal of Physical Chemistry Letters*, **2015**, 6, 1661-5	6.4	32
313	Cooperative Effects in Water Binding to Cuprous Oxide Surfaces. *Journal of Physical Chemistry C*, **2015**, 119, 9311-9323	3.8	31
312	Introducing PROFESS 3.0: An advanced program for orbital-free density functional theory molecular dynamics simulations. *Computer Physics Communications*, **2015**, 190, 228-230	4.2	48
311	Bond dissociation energies of C10 and C18 methyl esters from local multireference averaged-coupled pair functional theory. *Journal of Physical Chemistry A*, **2015**, 119, 3429-39	2.8	22
310	A Strategy to Stabilize Kesterite CZTS for High-Performance Solar Cells. *Chemistry of Materials*, **2015**, 27, 2920-2927	9.6	44
309	What Is the Role of Pyridinium in Pyridine-Catalyzed CO2 Reduction on p-GaP Photocathodes?. *Journal of the American Chemical Society*, **2015**, 137, 13248-51	16.4	52
308	Ab initio pressure-dependent reaction kinetics of methyl propanoate radicals. *Physical Chemistry Chemical Physics*, **2015**, 17, 31061-72	3.6	14
307	Density Fitting and Cholesky Decomposition of the Two-Electron Integrals in Local Multireference Configuration Interaction Theory. *Journal of Chemical Theory and Computation*, **2015**, 11, 5242-51	6.4	12
306	Structural and Electronic Features of β-Ni(OH)2and β-NiOOH from First Principles. *Journal of Physical Chemistry C*, **2015**, 119, 24315-24322	3.8	114

305	Ab Initio Unimolecular Reaction Kinetics of CH2C(?O)OCH3 and CH3C(?O)OCH2 Radicals. *Journal of Physical Chemistry A*, **2015**, 119, 10553-62	2.8	15
304	Influence of Weak Br□sted Acids on Electrocatalytic CO2 Reduction by Manganese and Rhenium Bipyridine Catalysts. *ACS Catalysis*, **2015**, 5, 900-908	13.1	97
303	Assessment of a semi integral-direct local multi-reference configuration interaction implementation employing shared-memory parallelization. *Computational and Theoretical Chemistry*, **2015**, 1051, 47-56	2	9
302	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	5.9	40
301	Reply to □Comment on □Single-point kinetic energy density functionals: A pointwise kinetic energy density analysis and numerical convergence investigation□□*Physical Review B*, **2015**, 92,	3.3	12
300	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	3.9	34
299	Numerical Challenges in a Cholesky-Decomposed Local Correlation Quantum Chemistry Framework **2015**, 59-91		4
298	Three-dimensional hole transport in nickel oxide by alloying with MgO or ZnO. *Journal of Applied Physics*, **2015**, 118, 185102	2.5	6
297	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	3.8	7
296	Liquid li structure and dynamics: A comparison between OFDFT and second nearest-neighbor embedded-atom method. *AICHE Journal*, **2015**, 61, 2841-2853	3.6	19
295	Ab Initio Kinetics of Hydrogen Abstraction from Methyl Acetate by Hydrogen, Methyl, Oxygen, Hydroxyl, and Hydroperoxy Radicals. *Journal of Physical Chemistry A*, **2015**, 119, 6377-90	2.8	34
294	Strategies to suppress cation vacancies in metal oxide alloys: consequences for solar energy conversion. *Journal of Materials Science*, **2015**, 50, 5715-5722	4.3	8
293	Single-point kinetic energy density functionals: A pointwise kinetic energy density analysis and numerical convergence investigation. *Physical Review B*, **2015**, 91,	3.3	38
292	Cluster Models for Studying CO2 Reduction on Semiconductor Photoelectrodes. *Topics in Catalysis*, **2015**, 58, 46-56	2.3	28
291	Size-extensivity-corrected multireference configuration interaction schemes to accurately predict bond dissociation energies of oxygenated hydrocarbons. *Journal of Chemical Physics*, **2014**, 140, 044317	3.9	75
290	Analysis of and remedies for unphysical ground states of the multireference averaged coupled-pair functional. *Journal of Chemical Physics*, **2014**, 140, 024102	3.9	6
289	First-principles simulations of plasticity in body-centered-cubic magnesium□thium alloys. *Acta Materialia*, **2014**, 64, 198-207	8.4	29
288	Enhanced von Weizs□ker Wang-Govind-Carter kinetic energy density functional for semiconductors. *Journal of Chemical Physics*, **2014**, 140, 18A531	3.9	50

287	Angular momentum dependent orbital-free density functional theory: Formulation and implementation. *Physical Review B*, **2014**, 89,	3.3	15
286	Status in calculating electronic excited states in transition metal oxides from first principles. *Topics in Current Chemistry*, **2014**, 347, 47-98		14
285	Oxygen transport in perovskite-type solid oxide fuel cell materials: insights from quantum mechanics. *Accounts of Chemical Research*, **2014**, 47, 3340-8	24.3	90
284	Ab initio DFT+U analysis of oxygen transport in LaCoO3: the effect of Co3+ magnetic states. *Journal of Materials Chemistry A*, **2014**, 2, 8060-8074	13	63
283	Mechanistic contrasts between manganese and rhenium bipyridine electrocatalysts for the reduction of carbon dioxide. *Journal of the American Chemical Society*, **2014**, 136, 16285-98	16.4	221
282	Accurate bond energies of biodiesel methyl esters from multireference averaged coupled-pair functional calculations. *Journal of Physical Chemistry A*, **2014**, 118, 7392-403	2.8	38
281	Trends in bond dissociation energies of alcohols and aldehydes computed with multireference averaged coupled-pair functional theory. *Journal of Physical Chemistry A*, **2014**, 118, 3039-50	2.8	27
280	Theoretical investigation of H2 oxidation on the Sr2Fe(1.5)Mo(0.5)O6 (001) perovskite surface under anodic solid oxide fuel cell conditions. *Journal of the American Chemical Society*, **2014**, 136, 8374-86	16.4	55
279	Embedded correlated wavefunction schemes: theory and applications. *Accounts of Chemical Research*, **2014**, 47, 2768-75	24.3	160
278	Revisiting photoemission and inverse photoemission spectra of nickel oxide from first principles: implications for solar energy conversion. *Journal of Physical Chemistry B*, **2014**, 118, 7963-71	3.4	32
277	Hydrogen-bonded cyclic water clusters nucleated on an oxide surface. *Journal of the American Chemical Society*, **2014**, 136, 13283-8	16.4	25
276	Titanium incorporation into hematite photoelectrodes: theoretical considerations and experimental observations. *Energy and Environmental Science*, **2014**, 7, 3100-3121	35.4	105
275	Simulations of dislocation mobility in magnesium from first principles. *International Journal of Plasticity*, **2014**, 60, 58-70	7.6	38
274	Orbital-free density functional theory study of crystalline Li–Si alloys. *Journal of Power Sources*, **2014**, 254, 62-72	8.9	16
273	First-Principles Study of Lanthanum Strontium Manganite: Insights into Electronic Structure and Oxygen Vacancy Formation. *Journal of Physical Chemistry C*, **2014**, 118, 13346-13356	3.8	67
272	Shared-memory parallelization of a local correlation multi-reference CI program. *Computer Physics Communications*, **2014**, 185, 3175-3188	4.2	8
271	First-Principles Modeling of Electrochemical Water Oxidation on MnO:ZnO(001). *ChemElectroChem*, **2014**, 1, 407-415	4.3	14
270	Communication: comparing ab initio methods of obtaining effective U parameters for closed-shell materials. *Journal of Chemical Physics*, **2014**, 140, 121105	3.9	47

269	Significant reduction in NiO band gap upon formation of Lix Ni1-x O alloys: applications to solar energy conversion. *ChemSusChem*, **2014**, 7, 195-201	8.3	45
268	Time-dependent potential-functional embedding theory. *Journal of Chemical Physics*, **2014**, 140, 124113	3.9	16
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