Emily Ann Carter

List of Publications by Citations

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	Hot electrons do the impossible: plasmon-induced dissociation of H2 on Au. *Nano Letters*, **2013**, 13, 240-7	11.5	1091
429	Constrained reaction coordinate dynamics for the simulation of rare events. *Chemical Physics Letters*, **1989**, 156, 472-477	2.5	726
428	Oligoacenes: theoretical prediction of open-shell singlet diradical ground states. *Journal of the American Chemical Society*, **2004**, 126, 7416-7	16.4	591
427	Quantifying hot carrier and thermal contributions in plasmonic photocatalysis. *Science*, **2018**, 362, 69-72	33.3	494
426	The technological and economic prospects for CO utilization and removal. *Nature*, **2019**, 575, 87-97	50.4	479
425	Water oxidation on pure and doped hematite (0001) surfaces: prediction of Co and Ni as effective dopants for electrocatalysis. *Journal of the American Chemical Society*, **2012**, 134, 13296-309	16.4	411
424	Solvation dynamics for an ion pair in a polar solvent: Time-dependent fluorescence and photochemical charge transfer. *Journal of Chemical Physics*, **1991**, 94, 5961-5979	3.9	379
423	Carbon dissolution and diffusion in ferrite and austenite from first principles. *Physical Review B*, **2003**, 67,	3.3	354
422	Diffusion of interstitial hydrogen into and through bcc Fe from first principles. *Physical Review B*, **2004**, 70,	3.3	323
421	First-principles study of the surfaces of zirconia. *Physical Review B*, **1998**, 58, 8050-8064	3.3	306
420	First principles scheme to evaluate band edge positions in potential transition metal oxide photocatalysts and photoelectrodes. *Physical Chemistry Chemical Physics*, **2011**, 13, 16644-54	3.6	287
419	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
418	Relation between singlet-triplet gaps and bond energies. *The Journal of Physical Chemistry*, **1986**, 90, 998-1001		241
417	Theoretical Insights into Heterogeneous (Photo)electrochemical CO Reduction. *Chemical Reviews*, **2019**, 119, 6631-6669	68.1	238
416	Rotationally invariant ab initio evaluation of Coulomb and exchange parameters for DFT+U calculations. *Journal of Chemical Physics*, **2008**, 129, 014103	3.9	236
415	Aluminum Nanocrystals as a Plasmonic Photocatalyst for Hydrogen Dissociation. *Nano Letters*, **2016**, 16, 1478-84	11.5	234
414	Electron transport in pure and doped hematite. *Nano Letters*, **2011**, 11, 1775-81	11.5	227

413	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
412	Light-driven methane dry reforming with single atomic site antenna-reactor plasmonic photocatalysts. *Nature Energy*, **2020**, 5, 61-70	62.3	213
411	Elucidation of the selectivity of proton-dependent electrocatalytic CO2 reduction by fac-Re(bpy)(CO)3Cl. *Journal of the American Chemical Society*, **2013**, 135, 15823-9	16.4	207
410	Quantum mechanical embedding theory based on a unique embedding potential. *Journal of Chemical Physics*, **2011**, 134, 154110	3.9	200
409	Challenges in modeling materials properties without experimental input. *Science*, **2008**, 321, 800-3	33.3	200
408	A quantum-mechanically informed continuum model of hydrogen embrittlement. *Journal of the Mechanics and Physics of Solids*, **2004**, 52, 2403-2430	5	200
407	New concepts and modeling strategies to design and evaluate photo-electro-catalysts based on transition metal oxides. *Chemical Society Reviews*, **2013**, 42, 2401-22	58.5	197
406	Hydrogen in tungsten: Absorption, diffusion, vacancy trapping, and decohesion. *Journal of Materials Research*, **2010**, 25, 315-327	2.5	194
405	Electronic-structure calculations by first-principles density-based embedding of explicitly correlated systems. *Journal of Chemical Physics*, **1999**, 110, 7677-7688	3.9	189
404	Advances in correlated electronic structure methods for solids, surfaces, and nanostructures. *Annual Review of Physical Chemistry*, **2008**, 59, 261-90	15.7	182
403	Orbital-free kinetic-energy density functionals with a density-dependent kernel. *Physical Review B*, **1999**, 60, 16350-16358	3.3	181
402	Solute-dependent solvent force constants for ion pairs and neutral pairs in a polar solvent. *The Journal of Physical Chemistry*, **1989**, 93, 2184-2187		177
401	Structure, bonding, and adhesion at the TiC(100)/Fe(110) interface from first principles. *Journal of Chemical Physics*, **2003**, 118, 8982-8996	3.9	169
400	Accurate ab initio energetics of extended systems via explicit correlation embedded in a density functional environment. *Chemical Physics Letters*, **1998**, 295, 129-134	2.5	163
399	First principles assessment of ideal fracture energies of materials with mobile impurities: implications for hydrogen embrittlement of metals. *Acta Materialia*, **2004**, 52, 4801-4807	8.4	162
398	Embedded correlated wavefunction schemes: theory and applications. *Accounts of Chemical Research*, **2014**, 47, 2768-75	24.3	160
397	Ab initio evaluation of Coulomb and exchange parameters for DFT+U calculations. *Physical Review B*, **2007**, 76,	3.3	151
396	Adsorption and diffusion energetics of hydrogen atoms on Fe(110) from first principles. *Surface Science*, **2003**, 547, 85-98	1.8	148

395	Theoretical insights into pyridinium-based photoelectrocatalytic reduction of CO2. *Journal of the American Chemical Society*, **2012**, 134, 7580-3	16.4	145
394	Correlation-consistent singlet□triplet gaps in substituted carbenes. *Journal of Chemical Physics*, **1988**, 88, 1752-1763	3.9	130
393	Unveiling structure-property relationships in Sr2Fe(1.5)Mo(0.5)O(6-□), an electrode material for symmetric solid oxide fuel cells. *Journal of the American Chemical Society*, **2012**, 134, 6826-33	16.4	127
392	Interatomic potentials for hydrogen in □□ron based on density functional theory. *Physical Review B*, **2009**, 79,	3.3	126
391	Ab Initio DFT+U Analysis of Oxygen Vacancy Formation and Migration in La1-xSrxFeO3-□(x = 0, 0.25, 0.50). *Chemistry of Materials*, **2013**, 25, 3011-3019	9.6	125
390	Adsorption of hydrogen atoms on the Si(100)-2□1 surface: implications for the H2 desorption mechanism. *Chemical Physics Letters*, **1991**, 185, 172-178	2.5	124
389	Carbon atom adsorption on and diffusion into Fe(110) and Fe(100) from first principles. *Physical Review B*, **2005**, 71,	3.3	122
388	Periodic density functional embedding theory for complete active space self-consistent field and configuration interaction calculations: Ground and excited states. *Journal of Chemical Physics*, **2002**, 116, 42	3.9	122
387	Testing variations of the GW approximation on strongly correlated transition metal oxides: hematite (□-Fe2O3) as a benchmark. *Physical Chemistry Chemical Physics*, **2011**, 13, 15189-99	3.6	120
386	Quantum-mechanics-based design principles for solid oxide fuel cell cathode materials. *Energy and Environmental Science*, **2011**, 4, 4933	35.4	118
385	Orbital-free kinetic-energy functionals for the nearly free electron gas. *Physical Review B*, **1998**, 58, 13465-13471	3.3	118
384	Kinetic and Mechanistic Effects of Bipyridine (bpy) Substituent, Labile Ligand, and Br□sted Acid on Electrocatalytic CO2 Reduction by Re(bpy) Complexes. *ACS Catalysis*, **2018**, 8, 2021-2029	13.1	117
383	CO2 Adsorption on Cu2O(111): A DFT+U and DFT-D Study. *Journal of Physical Chemistry C*, **2013**, 117, 26048-26059	3.8	116
382	Chemisorption of oxygen, chlorine, hydrogen, hydroxide, and ethylene on silver clusters: A model for the olefin epoxidation reaction. *Surface Science*, **1989**, 209, 243-289	1.8	115
381	Early- versus late-transition-metal-oxo bonds: the electronic structure of oxovanadium(1+) and oxoruthenium(1+). *The Journal of Physical Chemistry*, **1988**, 92, 2109-2115		115
380	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
379	Structural and Electronic Features of □Ni(OH)2and □NiOOH from First Principles. *Journal of Physical Chemistry C*, **2015**, 119, 24315-24322	3.8	114
378	Ridge method for finding saddle points on potential energy surfaces. *Journal of Chemical Physics*, **1993**, 98, 6377-6386	3.9	114

377	Self-consistent embedding theory for locally correlated configuration interaction wave functions in condensed matter. *Journal of Chemical Physics*, **2006**, 125, 084102	3.9	112
376	Structure and stability of Fe3C-cementite surfaces from first principles. *Surface Science*, **2003**, 530, 88-100	1.8	112
375	First-principles exploration of alternative gate dielectrics: Electronic structure of ZrO2/Si and ZrSiO4/Si interfaces. *Physical Review B*, **2004**, 69,	3.3	110
374	Origin of the energy barrier to chemical reactions of O2 on Al(111): evidence for charge transfer, not spin selection. *Physical Review Letters*, **2012**, 109, 198303	7.4	109
373	Importance of shear in the bcc-to-hcp transformation in iron. *Physical Review Letters*, **2004**, 93, 115501	7.4	109
372	Adsorption and dissociation of CO on Fe(1 1 0) from first principles. *Surface Science*, **2004**, 570, 167-177	1.8	108
371	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
370	Adhesion of ultrathin ZrO2(111) films on Ni(111) from first principles. *Journal of Chemical Physics*, **2001**, 114, 5816-5831	3.9	107
369	Ab initio molecular dynamics with correlated molecular wave functions: Generalized valence bond molecular dynamics and simulated annealing. *Journal of Chemical Physics*, **1992**, 97, 6569-6578	3.9	106
368	Titanium incorporation into hematite photoelectrodes: theoretical considerations and experimental observations. *Energy and Environmental Science*, **2014**, 7, 3100-3121	35.4	105
367	The electronic states of rhenium bipyridyl electrocatalysts for CO2 reduction as revealed by X-ray absorption spectroscopy and computational quantum chemistry. *Angewandte Chemie - International Edition*, **2013**, 52, 4841-4	16.4	105
366	Nonlocal orbital-free kinetic energy density functional for semiconductors. *Physical Review B*, **2010**, 81,	3.3	104
365	Electrochemical reactivities of pyridinium in solution: consequences for CO2 reduction mechanisms. *Chemical Science*, **2013**, 4, 1490	9.4	103
364	Response to Comment on "Quantifying hot carrier and thermal contributions in plasmonic photocatalysis". *Science*, **2019**, 364,	33.3	102
363	Band Gap Engineering of MnO via ZnO Alloying: A Potential New Visible-Light Photocatalyst. *Journal of Physical Chemistry C*, **2012**, 116, 9876-9887	3.8	101
362	Spin eigenstate-dependent Hartree–Fock molecular dynamics. *Chemical Physics Letters*, **1992**, 189, 358-362	2.5	101
361	Prediction of electronic excited states of adsorbates on metal surfaces from first principles. *Physical Review Letters*, **2001**, 86, 5954-7	7.4	100
360	Structure, bonding, and adhesion at the ZrC(1 0 0)/Fe(1 1 0) interface from first principles. *Surface Science*, **2004**, 560, 103-120	1.8	99

359	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
358	First-principles predictions of the structure, stability, and photocatalytic potential of Cu2O surfaces. *Journal of Physical Chemistry B*, **2013**, 117, 15750-60	3.4	93
357	Interactions of nitric oxide and carbon monoxide with palladium and platinum atoms. *The Journal of Physical Chemistry*, **1991**, 95, 2327-2339		93
356	Potential-functional embedding theory for molecules and materials. *Journal of Chemical Physics*, **2011**, 135, 194104	3.9	92
355	Adsorption of Al, O, Hf, Y, Pt, and S Atoms on □-Al2O3(0001). *Journal of Physical Chemistry C*, **2007**, 111, 7105-7126	3.8	92
354	Adsorption, Diffusion, and Dissociation of H2S on Fe(100) from First Principles. *Journal of Physical Chemistry B*, **2004**, 108, 19140-19145	3.4	92
353	Effect of Antisite Defects on the Formation of Oxygen Vacancies in Sr2FeMoO6: Implications for Ion and Electron Transport. *Chemistry of Materials*, **2011**, 23, 4525-4536	9.6	91
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350	Correlation-consistent configuration interaction: Accurate bond dissociation energies from simple wave functions. *Journal of Chemical Physics*, **1988**, 88, 3132-3140	3.9	89
349	Ab initio H2 desorption pathways for H/Si(100): the role of SiH2(a). *Surface Science*, **1993**, 295, 64-78	1.8	88
348	First-principles-derived dynamics of a surface reaction: Fluorine etching of Si(100). *Physical Review Letters*, **1992**, 69, 200-203	7.4	88
347	Importance of reference Hamiltonians containing exact exchange for accurate one-shot GW calculations of Cu2O. *Physical Review B*, **2012**, 85,	3.3	87
346	The surface atomic oxyradical mechanism for Ag-catalyzed olefin epoxidation*1. *Journal of Catalysis*, **1988**, 112, 80-92	7.3	85
345	Effects of segregating elements on the adhesive strength and structure of the □-Al2O3/╫NiAl interface. *Acta Materialia*, **2007**, 55, 2791-2803	8.4	84
344	Relationships between bond energies in coordinatively unsaturated and coordinatively saturated transition-metal complexes: a quantitative guide for single, double, and triple bonds. *The Journal of Physical Chemistry*, **1988**, 92, 5679-5683		84
343	Accurate simulations of metals at the mesoscale: Explicit treatment of 1 million atoms with quantum mechanics. *Chemical Physics Letters*, **2009**, 475, 163-170	2.5	83
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340	Plasmon damping depends on the chemical nature of the nanoparticle interface. *Science Advances*, **2019**, 5, eaav0704	14.3	80
339	Electronic effects of surface oxygen on the bonding of NO to Pt(111). *Surface Science*, **1989**, 219, 467-482	2.8	80
338	Electronic Structure of Pure and Doped Cuprous Oxide with Copper Vacancies: Suppression of Trap States. *Chemistry of Materials*, **2013**, 25, 253-265	9.6	79
337	Structures and adsorption energetics for chemisorbed fluorine atoms on Si(100)-2 x 1. *Physical Review B*, **1992**, 45, 9065-9081	3.3	78
336	Introducing PROFESS: A new program for orbital-free density functional theory calculations. *Computer Physics Communications*, **2008**, 179, 839-854	4.2	77
335	Finding transition states for crystalline solid-solid phase transformations. *Proceedings of the National Academy of Sciences of the United States of America*, **2005**, 102, 6738-43	11.5	77
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326	First principles study of H2S adsorption and dissociation on Fe(110). *Surface Science*, **2005**, 583, 60-68	1.8	68
325	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
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321	Surface chemical reactions studied via ab initio-derived molecular dynamics simulations: Fluorine etching of Si(100). *Journal of Chemical Physics*, **1993**, 98, 737-745	3.9	64
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302	Plasmonic Photocatalysis of Nitrous Oxide into N and O Using Aluminum-Iridium Antenna-Reactor Nanoparticles. *ACS Nano*, **2019**, 13, 8076-8086	16.7	55
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