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	Hot Electrons Do the Impossible: Plasmon-Induced Dissociation of H₂ on Au. Nano Letters, 2013, 13, 240-247.	4.5	1,332
2	The technological and economic prospects for CO2 utilization and removal. Nature, 2019, 575, 87-97.	13.7	1,142
3	Constrained reaction coordinate dynamics for the simulation of rare events. Chemical Physics Letters, 1989, 156, 472-477.	1.2	840
4	Quantifying hot carrier and thermal contributions in plasmonic photocatalysis. Science, 2018, 362, 69-72.	6.0	756
5	Oligoacenes:Â Theoretical Prediction of Open-Shell Singlet Diradical Ground States. Journal of the American Chemical Society, 2004, 126, 7416-7417.	6.6	655
6	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, 13296-13309.	6.6	492
7	Light-driven methane dry reforming with single atomic site antenna-reactor plasmonic photocatalysts. Nature Energy, 2020, 5, 61-70.	19.8	466
8	Theoretical Insights into Heterogeneous (Photo)electrochemical CO₂Reduction. Chemical Reviews, 2019, 119, 6631-6669.	23.0	431
9	Diffusion of interstitial hydrogen into and through bcc Fe from first principles. Physical Review B, 2004, 70, .	1.1	406
10	Carbon dissolution and diffusion in ferrite and austenite from first principles. Physical Review B, 2003, 67, .	1.1	398
11	Solvation dynamics for an ion pair in a polar solvent: Timeâ€dependent fluorescence and photochemical charge transfer. Journal of Chemical Physics, 1991, 94, 5961-5979.	1.2	396
12	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
13	First principles scheme to evaluate band edge positions in potential transition metal oxide photocatalysts and photoelectrodes. Physical Chemistry Chemical Physics, 2011, 13, 16644.	1.3	380
14	First-principles study of the surfaces of zirconia. Physical Review B, 1998, 58, 8050-8064.	1.1	349
15	Aluminum Nanocrystals as a Plasmonic Photocatalyst for Hydrogen Dissociation. Nano Letters, 2016, 16, 1478-1484.	4.5	294
16	Relation between singlet-triplet gaps and bond energies. The Journal of Physical Chemistry, 1986, 90, 998-1001.	2.9	283
17	Rotationally invariant ab initio evaluation of Coulomb and exchange parameters for DFT+U calculations. Journal of Chemical Physics, 2008, 129, 014103.	1.2	282
18	Mechanistic Contrasts between Manganese and Rhenium Bipyridine Electrocatalysts for the Reduction of Carbon Dioxide. Journal of the American Chemical Society, 2014, 136, 16285-16298.	6.6	269

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19	Electron Transport in Pure and Doped Hematite. Nano Letters, 2011, 11, 1775-1781.	4.5	267
20	A quantum-mechanically informed continuum model of hydrogen embrittlement. Journal of the Mechanics and Physics of Solids, 2004, 52, 2403-2430.	2.3	246
21	Elucidation of the Selectivity of Proton-Dependent Electrocatalytic CO₂ Reduction by fac-Re(bpy)(CO)₃Cl. Journal of the American Chemical Society, 2013, 135, 15823-15829.	6.6	238
22	Quantum mechanical embedding theory based on a unique embedding potential. Journal of Chemical Physics, 2011, 134, 154110.	1.2	236
23	Hydrogen in tungsten: Absorption, diffusion, vacancy trapping, and decohesion. Journal of Materials Research, 2010, 25, 315-327.	1.2	230
24	New concepts and modeling strategies to design and evaluate photo-electro-catalysts based on transition metal oxides. Chemical Society Reviews, 2013, 42, 2401-2422.	18.7	225
25	Challenges in Modeling Materials Properties Without Experimental Input. Science, 2008, 321, 800-803.	6.0	222
26	Electronic-structure calculations by first-principles density-based embedding of explicitly correlated systems. Journal of Chemical Physics, 1999, 110, 7677-7688.	1.2	216
27	Orbital-free kinetic-energy density functionals with a density-dependent kernel. Physical Review B, 1999, 60, 16350-16358.	1.1	212
28	Advances in Correlated Electronic Structure Methods for Solids, Surfaces, and Nanostructures. Annual Review of Physical Chemistry, 2008, 59, 261-290.	4.8	210
29	Embedded Correlated Wavefunction Schemes: Theory and Applications. Accounts of Chemical Research, 2014, 47, 2768-2775.	7.6	205
30	Ab initioevaluation of Coulomb and exchange parameters for<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:mi>DFT</mml:mi><mml:mo>+</mml:mo><mml:mi mathvariant="normal">U</mml:mi></mml:mrow></mml:math>calculations. Physical Review B, 2007, 76, .	1.1	195
31	First principles assessment of ideal fracture energies of materials with mobile impurities: implications for hydrogen embrittlement of metals. Acta Materialia, 2004, 52, 4801-4807.	3.8	191
32	Accurate ab initio energetics of extended systems via explicit correlation embedded in a density functional environment. Chemical Physics Letters, 1998, 295, 129-134.	1.2	189
33	Solute-dependent solvent force constants for ion pairs and neutral pairs in a polar solvent. The Journal of Physical Chemistry, 1989, 93, 2184-2187.	2.9	188
34	Structure, bonding, and adhesion at the TiC(100)/Fe(110) interface from first principles. Journal of Chemical Physics, 2003, 118, 8982-8996.	1.2	183
35	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
36	Unveiling Structureâ€“Property Relationships in Sr₂Fe_{1.5}Mo_{0.5}O_{6â^'Î´}, an Electrode Material for Symmetric Solid Oxide Fuel Cells. Journal of the American Chemical Society, 2012, 134, 6826-6833.	6.6	172

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37	Interatomic potentials for hydrogen in<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mi>Î±</mml:mi></mml:math>â€“iron based on density functional theory. Physical Review B, 2009, 79, .	1.1	166
38	Adsorption and diffusion energetics of hydrogen atoms on Fe(110) from first principles. Surface Science, 2003, 547, 85-98.	0.8	161
39	Theoretical Insights into Pyridinium-Based Photoelectrocatalytic Reduction of CO₂. Journal of the American Chemical Society, 2012, 134, 7580-7583.	6.6	161
40	CO₂ Adsorption on Cu₂O(111): A DFT+U and DFT-D Study. Journal of Physical Chemistry C, 2013, 117, 26048-26059.	1.5	161
41	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
42	Ab Initio DFT+U Analysis of Oxygen Vacancy Formation and Migration in La_{1-x}Sr_xFeO_{3-Î´}(x= 0, 0.25, 0.50). Chemistry of Materials, 2013, 25, 3011-3019.	3.2	153
43	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
44	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
45	Correlationâ€consistent singletâ€“triplet gaps in substituted carbenes. Journal of Chemical Physics, 1988, 88, 1752-1763.	1.2	144
46	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.	1.2	142
47	Quantum-mechanics-based design principles for solid oxide fuel cell cathode materials. Energy and Environmental Science, 2011, 4, 4933.	15.6	141
48	Orbital-free kinetic-energy functionals for the nearly free electron gas. Physical Review B, 1998, 58, 13465-13471.	1.1	139
49	Carbon atom adsorption on and diffusion into Fe(110) and Fe(100) from first principles. Physical Review B, 2005, 71, .	1.1	136
50	Testing variations of the GW approximation on strongly correlated transition metal oxides: hematite (Î±-Fe2O3) as a benchmark. Physical Chemistry Chemical Physics, 2011, 13, 15189.	1.3	135
51	Importance of Shear in the bcc-to-hcp Transformation in Iron. Physical Review Letters, 2004, 93, 115501.	2.9	133
52	Chemisorption of oxygen, chlorine, hydrogen, hydroxide, and ethylene on silver clusters: A model for the olefin epoxidation reaction. Surface Science, 1989, 209, 243-289.	0.8	131
53	Adsorption of hydrogen atoms on the Si(100)-2Ã—1 surface: implications for the H2 desorption mechanism. Chemical Physics Letters, 1991, 185, 172-178.	1.2	131
54	Ridge method for finding saddle points on potential energy surfaces. Journal of Chemical Physics, 1993, 98, 6377-6386.	1.2	131

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55	Response to Comment on â€œQuantifying hot carrier and thermal contributions in plasmonic photocatalysisâ€. Science, 2019, 364, .	6.0	131
56	Structure and stability of Fe3C-cementite surfaces from first principles. Surface Science, 2003, 530, 88-100.	0.8	130
57	Nonlocal orbital-free kinetic energy density functional for semiconductors. Physical Review B, 2010, 81, .	1.1	128
58	Plasmon damping depends on the chemical nature of the nanoparticle interface. Science Advances, 2019, 5, eaav0704.	4.7	128
59	Self-consistent embedding theory for locally correlated configuration interaction wave functions in condensed matter. Journal of Chemical Physics, 2006, 125, 084102.	1.2	126
60	Origin of the Energy Barrier to Chemical Reactions of<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:msub><mml:mi mathvariant="normal">O</mml:mi><mml:mn>2</mml:mn></mml:msub></mml:math>on Al(111): Evidence for Charge Transfer, Not Spin Selection. Physical Review Letters, 2012, 109, 198303.	2.9	125
61	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.	2.9	124
62	Oxygen Transport in Perovskite-Type Solid Oxide Fuel Cell Materials: Insights from Quantum Mechanics. Accounts of Chemical Research, 2014, 47, 3340-3348.	7.6	121
63	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
64	The Electronic States of Rhenium Bipyridyl Electrocatalysts for CO₂ Reduction as Revealed by Xâ€ray Absorption Spectroscopy and Computational Quantum Chemistry. Angewandte Chemie - International Edition, 2013, 52, 4841-4844.	7.2	119
65	Adsorption and dissociation of CO on Fe(110) from first principles. Surface Science, 2004, 570, 167-177.	0.8	118
66	Importance of reference Hamiltonians containing exact exchange for accurate one-shot<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:mi>G</mml:mi><mml:mi>W</mml:mi></mml:mrow></mml:math>calculations of Cu<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:msub><mml:mrow /><mml:mn>2</mml:mn></mml:msub></mml:math>O. Physical Review B, 2012, 85, .	1.1	118
67	Band Gap Engineering of MnO via ZnO Alloying: A Potential New Visible-Light Photocatalyst. Journal of Physical Chemistry C, 2012, 116, 9876-9887.	1.5	118
68	Titanium incorporation into hematite photoelectrodes: theoretical considerations and experimental observations. Energy and Environmental Science, 2014, 7, 3100-3121.	15.6	118
69	First-principles exploration of alternative gate dielectrics:â€ƒElectronic structure ofZrO2/SiandZrSiO4/Siinterfaces. Physical Review B, 2004, 69, .	1.1	116
70	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.	1.2	115
71	First-Principles Predictions of the Structure, Stability, and Photocatalytic Potential of Cu₂O Surfaces. Journal of Physical Chemistry B, 2013, 117, 15750-15760.	1.2	115
72	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

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73	Adhesion of ultrathin ZrO2(111) films on Ni(111) from first principles. Journal of Chemical Physics, 2001, 114, 5816-5831.	1.2	112
74	Prediction of Electronic Excited States of Adsorbates on Metal Surfaces from First Principles. Physical Review Letters, 2001, 86, 5954-5957.	2.9	111
75	Electrochemical reactivities of pyridinium in solution: consequences for CO2 reduction mechanisms. Chemical Science, 2013, 4, 1490.	3.7	110
76	A Density Functional +UAssessment of Oxygen Evolution Reaction Mechanisms on Î²-NiOOH. ACS Catalysis, 2017, 7, 5329-5339.	5.5	110
77	Orbital-free density functional theory for materials research. Journal of Materials Research, 2018, 33, 777-795.	1.2	109
78	Structure, bonding, and adhesion at the ZrC(100)/Fe(110) interface from first principles. Surface Science, 2004, 560, 103-120.	0.8	108
79	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.	3.2	108
80	Potential-functional embedding theory for molecules and materials. Journal of Chemical Physics, 2011, 135, 194104.	1.2	108
81	Spin eigenstate-dependent Hartreeâ€"Fock molecular dynamics. Chemical Physics Letters, 1992, 189, 358-362.	1.2	106
82	Transferable local pseudopotentials for magnesium, aluminum and silicon. Physical Chemistry Chemical Physics, 2008, 10, 7109.	1.3	106
83	Interactions of nitric oxide and carbon monoxide with palladium and platinum atoms. The Journal of Physical Chemistry, 1991, 95, 2327-2339.	2.9	105
84	Adsorption, Diffusion, and Dissociation of H2S on Fe(100) from First Principles. Journal of Physical Chemistry B, 2004, 108, 19140-19145.	1.2	101
85	Adsorption of Al, O, Hf, Y, Pt, and S Atoms on Î±-Al2O3(0001). Journal of Physical Chemistry C, 2007, 111, 7105-7126.	1.5	101
86	Effects of segregating elements on the adhesive strength and structure of the Î±-Al2O3/Î²-NiAl interface. Acta Materialia, 2007, 55, 2791-2803.	3.8	100
87	Electronic Structure of Pure and Doped Cuprous Oxide with Copper Vacancies: Suppression of Trap States. Chemistry of Materials, 2013, 25, 253-265.	3.2	98
88	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, .	0.0	97
89	Accurate simulations of metals at the mesoscale: Explicit treatment of 1 million atoms with quantum mechanics. Chemical Physics Letters, 2009, 475, 163-170.	1.2	96
90	Correlationâ€consistent configuration interaction: Accurate bond dissociation energies from simple wave functions. Journal of Chemical Physics, 1988, 88, 3132-3140.	1.2	95

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91	A method for estimating surface reaction energetics: Application to the mechanism of ethylene decomposition on Pt(111). Surface Science, 1990, 226, 339-357.	0.8	95
92	Finding transition states for crystalline solid-solid phase transformations. Proceedings of the National Academy of Sciences of the United States of America, 2005, 102, 6738-6743.	3.3	95
93	The surface atomic oxyradical mechanism for Ag-catalyzed olefin epoxidation*1. Journal of Catalysis, 1988, 112, 80-92.	3.1	94
94	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.	2.9	93
95	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
96	First-principles-derived dynamics of a surface reaction: Fluorine etching of Si(100). Physical Review Letters, 1992, 69, 200-203.	2.9	91
97	Ab initio H2 desorption pathways for H/Si(100): the role of SiH2(a). Surface Science, 1993, 295, 64-78.	0.8	91
98	Introducing PROFESS: A new program for orbital-free density functional theory calculations. Computer Physics Communications, 2008, 179, 839-854.	3.0	90
99	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
100	Improving the orbital-free density functional theory description of covalent materials. Journal of Chemical Physics, 2005, 122, 044103.	1.2	85
101	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
102	Electronic effects of surface oxygen on the bonding of NO to Pt(111). Surface Science, 1989, 219, 467-489.	0.8	84
103	Hole transport in pure and doped hematite. Journal of Applied Physics, 2012, 112, .	1.1	84
104	Long Live Vinylidene! A New View of the H2CC:â€‰ â†’ HCâ‹®CH Rearrangement from ab Initio Molecular Dynamics. Journal of the American Chemical Society, 2001, 123, 641-657.	6.6	83
105	Surface Energy as a Descriptor of Catalytic Activity. Journal of Physical Chemistry C, 2016, 120, 23698-23706.	1.5	83
106	Plasmonic Photocatalysis of Nitrous Oxide into N₂ and O₂ Using Aluminumâ€“Iridium Antennaâ€“Reactor Nanoparticles. ACS Nano, 2019, 13, 8076-8086.	7.3	83
107	First-Principles Study of Lanthanum Strontium Manganite: Insights into Electronic Structure and Oxygen Vacancy Formation. Journal of Physical Chemistry C, 2014, 118, 13346-13356.	1.5	82
108	Quantum Chemical Benchmarking, Validation, and Prediction of Acidity Constants for Substituted Pyridinium Ions and Pyridinyl Radicals. Journal of Chemical Theory and Computation, 2012, 8, 3187-3206.	2.3	81

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109	Defect-Mediated Charge-Carrier Trapping and Nonradiative Recombination in WSe₂ Monolayers. Journal of the American Chemical Society, 2019, 141, 10451-10461.	6.6	81
110	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
111	Structures and adsorption energetics for chemisorbed fluorine atoms on Si(100)-2Ã—1. Physical Review B, 1992, 45, 9065-9081.	1.1	80
112	Ab Initio Structure and Energetics for the Molecular and Dissociative Adsorption of NH3 on Si(100)-2 Ã— 1. Journal of Physical Chemistry B, 1997, 101, 8658-8661.	1.2	77
113	Transferable local pseudopotentials derived via inversion of the Kohn-Sham equations in a bulk environment. Physical Review B, 2004, 69, .	1.1	77
114	Thermochemistry of the selective dehydrogenation of cyclohexane to benzene on Pt surfaces. Journal of Molecular Catalysis A, 1998, 131, 39-53.	4.8	76
115	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.	5.2	76
116	Excited-State N₂ Dissociation Pathway on Fe-Functionalized Au. Journal of the American Chemical Society, 2017, 139, 4390-4398.	6.6	76
117	Understanding the Effects of Cd and Ag Doping in Cu₂ZnSnS₄ Solar Cells. Chemistry of Materials, 2018, 30, 4543-4555.	3.2	76
118	A dynamically and kinetically consistent mechanism forH2adsorption/desorption from Si(100)-2Ã—1. Physical Review B, 1996, 54, 11803-11817.	1.1	75
119	First principles study of H2S adsorption and dissociation on Fe(110). Surface Science, 2005, 583, 60-68.	0.8	75
120	Factors Governing Oxygen Vacancy Formation in Oxide Perovskites. Journal of the American Chemical Society, 2021, 143, 13212-13227.	6.6	75
121	Linear scaling multireference singles and doubles configuration interaction. Journal of Chemical Physics, 2008, 128, 224106.	1.2	74
122	Can orbital-free density functional theory simulate molecules?. Journal of Chemical Physics, 2012, 136, 084102.	1.2	74
123	Prediction of a low-temperature N ₂ dissociation catalyst exploiting near-IRâ€“toâ€“visible light nanoplasmonics. Science Advances, 2017, 3, eaao4710.	4.7	74
124	How To Identify Plasmons from the Optical Response of Nanostructures. ACS Nano, 2017, 11, 7321-7335.	7.3	72
125	Pseudospectral Mo/llerâ€“Plesset perturbation theory through third order. Journal of Chemical Physics, 1994, 100, 3631-3638.	1.2	70
126	Bonding in transition-metal-methylene complexes. 2. (RuCH2)+, a complex exhibiting low-lying methylidene-like and carbene-like states. Journal of the American Chemical Society, 1986, 108, 2180-2191.	6.6	69

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127	New predictions for singlet-triplet gaps of substituted carbenes. The Journal of Physical Chemistry, 1987, 91, 4651-4652.	2.9	69
128	Time-reversible multiple time scale ab initio molecular dynamics. The Journal of Physical Chemistry, 1993, 97, 13429-13434.	2.9	69
129	Surface chemical reactions studied via ab initioâ€derived molecular dynamics simulations: Fluorine etching of Si(100). Journal of Chemical Physics, 1993, 98, 737-745.	1.2	68
130	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, 8374-8386.	6.6	68
131	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
132	Energetics and kinetics of vacancy diffusion and aggregation in shocked aluminium via orbital-free density functional theory. Physical Chemistry Chemical Physics, 2007, 9, 4951.	1.3	65
133	Suppressed Deep Traps and Bandgap Fluctuations in Cu₂CdSnS₄ Solar Cells with â‰ˆ8% Efficiency. Advanced Energy Materials, 2019, 9, 1902509.	10.2	65
134	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
135	AB INITIO DYNAMICS OF SURFACE CHEMISTRY. Annual Review of Physical Chemistry, 1997, 48, 243-270.	4.8	64
136	Hybrid Density Functional Theory Predictions of Low-Temperature Dimethyl Ether Combustion Pathways. II. Chain-Branching Energetics and Possible Role of the Criegee Intermediate. Journal of Physical Chemistry A, 2003, 107, 9463-9478.	1.1	64
137	Density-functional-theory-based local quasicontinuum method: Prediction of dislocation nucleation. Physical Review B, 2004, 70, .	1.1	64
138	Universal binding-energy relation for crystals that accounts for surface relaxation. Physical Review B, 2004, 69, .	1.1	64
139	Transition metal oxide alloys as potential solar energy conversion materials. Journal of Materials Chemistry A, 2013, 1, 2474.	5.2	63
140	A Strategy to Stabilize Kesterite CZTS for High-Performance Solar Cells. Chemistry of Materials, 2015, 27, 2920-2927.	3.2	63
141	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
142	Subpicosecond interconversion of buckled and symmetric dimers on Si(100). Surface Science, 1990, 232, L219-L223.	0.8	62
143	Metallic Character of the Al2O3(0001)-(âˆš31 Ã— âˆš31)R Â± 9Â° Surface Reconstruction. Journal of Physical Chemistry B, 2001, 105, 4045-4052.	1.2	62
144	Local correlation in the virtual space in multireference singles and doubles configuration interaction. Journal of Chemical Physics, 2003, 118, 8127-8139.	1.2	62

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145	Mechanistic Insights into Photocatalyzed Hydrogen Desorption from Palladium Surfaces Assisted by Localized Surface Plasmon Resonances. ACS Nano, 2018, 12, 3512-3522.	7.3	62
146	Bonding in transition-metal methylene complexes. 3. Comparison of chromium and rubidium carbenes: prediction of stable LnM(CXY) systems. Journal of the American Chemical Society, 1986, 108, 4746-4754.	6.6	61
147	First-principles characterization of a heteroceramic interface:ZrO2(001)deposited on anÎ±â^'Al2O3(11Â¯02)substrate. Physical Review B, 2000, 62, 16968-16983.	1.1	61
148	Orbital-Free Kinetic-Energy Density Functional Theory. , 2002, , 117-184.		61
149	Communication: Comparing ab initio methods of obtaining effective U parameters for closed-shell materials. Journal of Chemical Physics, 2014, 140, 121105.	1.2	61
150	Linear-scaling parallel algorithms for the first principles treatment of metals. Computer Physics Communications, 2000, 128, 67-92.	3.0	60
151	A comparison of Carâ€"Parrinello and Bornâ€"Oppenheimer generalized valence bond molecular dynamics. Chemical Physics Letters, 1995, 240, 261-267.	1.2	59
152	Oxide ion transport in Sr2Fe1.5Mo0.5O6â^'Î´, a mixed ion-electron conductor: new insights from first principles modeling. Physical Chemistry Chemical Physics, 2013, 15, 6250.	1.3	59
153	Enhanced von WeizsÃcker Wang-Govind-Carter kinetic energy density functional for semiconductors. Journal of Chemical Physics, 2014, 140, 18A531.	1.2	59
154	Optical Excitations in Hematite (Î±-Fe₂O₃) via Embedded Cluster Models: A CASPT2 Study. Journal of Physical Chemistry C, 2011, 115, 20795-20805.	1.5	57
155	Theoretical Insights into Electrochemical CO₂ Reduction Mechanisms Catalyzed by Surface-Bound Nitrogen Heterocycles. Journal of Physical Chemistry Letters, 2013, 4, 4058-4063.	2.1	57
156	The chromium methylidene cation: CrCH2+. The Journal of Physical Chemistry, 1984, 88, 1485-1490.	2.9	56
157	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
158	First-principles-derived rate constants for H adatom surface diffusion on Si(100)-2Ã—1. Physical Review B, 1994, 49, 13488-13500.	1.1	55
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