John R Kitchin

List of Publications by Year
in descending order

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96 papers	25,489 citations	81900 39 h-index	39675 94 g-index

105 all docs	105 docs citations	105 times ranked	22783 citing authors

#	Article	IF	Citations
1	Origin of the Overpotential for Oxygen Reduction at a Fuel-Cell Cathode. Journal of Physical Chemistry B, 2004, 108, 17886-17892.	2.6	8,672
2	Trends in the Exchange Current for Hydrogen Evolution. Journal of the Electrochemical Society, 2005, 152, J23.	2.9	4,054
3	Universality in Oxygen Evolution Electrocatalysis on Oxide Surfaces. ChemCatChem, 2011, 3, 1159-1165.	3.7	3,208
4	The atomic simulation environmentâ€”a Python library for working with atoms. Journal of Physics Condensed Matter, 2017, 29, 273002.	1.8	1,933
5	Role of Strain and Ligand Effects in the Modification of the Electronic and Chemical Properties of Bimetallic Surfaces. Physical Review Letters, 2004, 93, 156801.	7.8	1,224
6	Modification of the surface electronic and chemical properties of Pt(111) by subsurface 3d transition metals. Journal of Chemical Physics, 2004, 120, 10240-10246.	3.0	1,181
7	The outlook for improved carbon capture technology. Progress in Energy and Combustion Science, 2012, 38, 630-671.	31.2	427
8	Spectroscopic Characterization of Mixed Feâ€“Ni Oxide Electrocatalysts for the Oxygen Evolution Reaction in Alkaline Electrolytes. ACS Catalysis, 2012, 2, 1793-1801.	11.2	423
9	Machine learning in catalysis. Nature Catalysis, 2018, 1, 230-232.	34.4	308
10	Trends in the chemical properties of early transition metal carbide surfaces: A density functional study. Catalysis Today, 2005, 105, 66-73.	4.4	302
11	Number of outer electrons as descriptor for adsorption processes on transition metals and their oxides. Chemical Science, 2013, 4, 1245.	7.4	273
12	Hydrogen Dissociation and Spillover on Individual Isolated Palladium Atoms. Physical Review Letters, 2009, 103, 246102.	7.8	216
13	Toward Benchmarking in Catalysis Science: Best Practices, Challenges, and Opportunities. ACS Catalysis, 2016, 6, 2590-2602.	11.2	190
14	Elucidation of the active surface and origin of the weak metalâ€“hydrogen bond on Ni/Pt(111) bimetallic surfaces: a surface science and density functional theory study. Surface Science, 2003, 544, 295-308.	1.9	154
15	Alloy surface segregation in reactive environments: First-principles atomistic thermodynamics study of<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:msub><mml:mi>Ag</mml:mi><mml:mn>3</mml:mn></mml:msub><mml:mi>Pd</mml:mi><mml:m oxygen atmospheres. Physical Review B, 2008, 77, .	3.2	129
16	Investigating the Reactivity of Single Atom Alloys Using Density Functional Theory. Topics in Catalysis, 2018, 61, 462-474.	2.8	117
17	Alkaline Electrolyte and Fe Impurity Effects on the Performance and Active-Phase Structure of NiOOH Thin Films for OER Catalysis Applications. Journal of Physical Chemistry C, 2015, 119, 11475-11481.	3.1	110
18	Effects of Concentration, Crystal Structure, Magnetism, and Electronic Structure Method on First-Principles Oxygen Vacancy Formation Energy Trends in Perovskites. Journal of Physical Chemistry C, 2014, 118, 28776-28790.	3.1	105

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19	Relating the coverage dependence of oxygen adsorption on Au and Pt fcc(111) surfaces through adsorbate-induced surface electronic structure effects. Surface Science, 2009, 603, 794-801.	1.9	97
20	Evaluation of a Primary Amine-Functionalized Ion-Exchange Resin for CO₂ Capture. Industrial & Engineering Chemistry Research, 2012, 51, 6907-6915.	3.7	97
21	pybliometrics: Scriptable bibliometrics using a Python interface to Scopus. SoftwareX, 2019, 10, 100263.	2.6	96
22	Correlations in coverage-dependent atomic adsorption energies on Pd(111). Physical Review B, 2009, 79, .	3.2	87
23	A Linear Response DFT+U Study of Trends in the Oxygen Evolution Activity of Transition Metal Rutile Dioxides. Journal of Physical Chemistry C, 2015, 119, 4827-4833.	3.1	86
24	Investigating the Energetic Ordering of Stable and Metastable TiO₂ Polymorphs Using DFT+U and Hybrid Functionals. Journal of Physical Chemistry C, 2015, 119, 21060-21071.	3.1	81
25	The Role of Adsorbateâ€“Adsorbate Interactions in the Rate Controlling Step and the Most Abundant Reaction Intermediate of NH₃Decomposition on Ru. Catalysis Letters, 2004, 96, 13-22.	2.6	76
26	Electrocatalytic Oxygen Evolution with an Immobilized TAML Activator. Journal of the American Chemical Society, 2014, 136, 5603-5606.	13.7	71
27	Quantifying Uncertainty in Activity Volcano Relationships for Oxygen Reduction Reaction. ACS Catalysis, 2016, 6, 5251-5259.	11.2	70
28	Effects of O₂ and SO₂ on the Capture Capacity of a Primary-Amine Based Polymeric CO₂ Sorbent. Industrial & Engineering Chemistry Research, 2013, 52, 10788-10794.	3.7	68
29	Effects of strain, d-band filling, and oxidation state on the surface electronic structure and reactivity of 3d perovskite surfaces. Journal of Chemical Physics, 2012, 137, 084703.	3.0	67
30	Neural network and ReaxFF comparison for Au properties. International Journal of Quantum Chemistry, 2016, 116, 979-987.	2.0	66
31	Simple model explaining and predicting coverage-dependent atomic adsorption energies on transition metal surfaces. Physical Review B, 2010, 82, .	3.2	62
32	Configurational correlations in the coverage dependent adsorption energies of oxygen atoms on late transition metal fcc(111) surfaces. Journal of Chemical Physics, 2011, 134, 104709.	3.0	58
33	Neural network predictions of oxygen interactions on a dynamic Pd surface. Molecular Simulation, 2017, 43, 346-354.	2.0	58
34	Separation of CO2 from flue gas using electrochemical cells. Fuel, 2010, 89, 1307-1314.	6.4	52
35	Redox-Mediated Separation of Carbon Dioxide from Flue Gas. Energy & Fuels, 2015, 29, 7508-7515.	5.1	48
36	Modeling Segregation on AuPd(111) Surfaces with Density Functional Theory and Monte Carlo Simulations. Journal of Physical Chemistry C, 2017, 121, 3479-3487.	3.1	48

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37	Alchemical Predictions for Computational Catalysis: Potential and Limitations. Journal of Physical Chemistry Letters, 2017, 8, 5002-5007.	4.6	48
38	Comparisons of amine solvents for post-combustion CO2 capture: A multi-objective analysis approach. International Journal of Greenhouse Gas Control, 2013, 18, 68-74.	4.6	46
39	Atomistic thermodynamics study of the adsorption and the effects of waterâ€“gas shift reactants on Cu catalysts under reaction conditions. Journal of Catalysis, 2009, 261, 188-194.	6.2	41
40	Parallelized Screening of Characterized and DFT-Modeled Bimetallic Colloidal Cocatalysts for Photocatalytic Hydrogen Evolution. ACS Catalysis, 2020, 10, 4244-4252.	11.2	41
41	A comparison of gold and molybdenum nanoparticles on TiO2() 1Ã—2 reconstructed single crystal surfaces. Surface Science, 2003, 526, 323-331.	1.9	38
42	New solid-state table: estimating d-band characteristics for transition metal atoms. Molecular Simulation, 2010, 36, 633-638.	2.0	37
43	Uncertainty and figure selection for DFT based cluster expansions for oxygen adsorption on Au and Pt (111) surfaces. Molecular Simulation, 2009, 35, 920-927.	2.0	35
44	Preparation and Characterization of a Bis-Semiquinone: a Bidentate Dianion Biradical. Journal of Organic Chemistry, 1995, 60, 3578-3579.	3.2	34
45	CO₂ Adsorption on Supported Molecular Amidine Systems on Activated Carbon. ChemSusChem, 2010, 3, 948-956.	6.8	32
46	Interactions in 1-ethyl-3-methyl imidazolium tetracyanoborate ion pair: Spectroscopic and density functional study. Journal of Molecular Structure, 2013, 1038, 12-18.	3.6	31
47	Tuning oxide activity through modification of the crystal and electronic structure: from strain to potential polymorphs. Physical Chemistry Chemical Physics, 2015, 17, 28943-28949.	2.8	31
48	Response to â€œComment on â€˜Trends in the Exchange Current for Hydrogen Evolutionâ€™ [J. Electrochem. Soc., 152, J23 (2005)]â€• Journal of the Electrochemical Society, 2006, 153, L33.	2.9	29
49	Probing the Coverage Dependence of Site and Adsorbate Configurational Correlations on (111) Surfaces of Late Transition Metals. Journal of Physical Chemistry C, 2014, 118, 25597-25602.	3.1	29
50	Relationships between the surface electronic and chemical properties of doped 4d and 5d late transition metal dioxides. Journal of Chemical Physics, 2015, 142, 104703.	3.0	28
51	Step decoration of chiral metal surfaces. Journal of Chemical Physics, 2009, 130, 124710.	3.0	27
52	Accurate electronic and chemical properties of 3d transition metal oxides using a calculated linear response U and a DFT + U(V) method. Journal of Chemical Physics, 2015, 142, 144701.	3.0	27
53	Machine-learning accelerated geometry optimization in molecular simulation. Journal of Chemical Physics, 2021, 154, 234704.	3.0	27
54	Identifying Potential BO₂ Oxide Polymorphs for Epitaxial Growth Candidates. ACS Applied Materials & Interfaces, 2014, 6, 3630-3639.	8.0	26

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55	SingleNN: Modified Behlerâ€“Parrinello Neural Network with Shared Weights for Atomistic Simulations with Transferability. Journal of Physical Chemistry C, 2020, 124, 17811-17818.	3.1	26
56	Preparation of Paramagnetic Ligands for Coordination-Complexes and Networks with Interesting Magnetic Properties. Molecular Crystals and Liquid Crystals, 1997, 305, 303-310.	0.3	25
57	Competitive Growth of Scrutinyite (Î±-PbO₂) and Rutile Polymorphs of SnO₂ on All Orientations of Columbite CoNb₂O₆ Substrates. Crystal Growth and Design, 2017, 17, 3929-3939.	3.0	25
58	Identification of Sulfur-Tolerant Bimetallic Surfaces Using DFT Parametrized Models and Atomistic Thermodynamics. ACS Catalysis, 2011, 1, 399-407.	11.2	24
59	Chemical and Molecular Descriptors for the Reactivity of Amines with CO₂. Industrial & Engineering Chemistry Research, 2012, 51, 13609-13618.	3.7	24
60	Estimating Bulk-Composition-Dependent H₂ Adsorption Energies on Cu_xPd_{1â€“x} Alloy (111) Surfaces. ACS Catalysis, 2015, 5, 1020-1026.	11.2	24
61	Electrochemical Concentration of Carbon Dioxide from an Oxygen/Carbon Dioxide Containing Gas Stream. Journal of the Electrochemical Society, 2010, 157, B1149.	2.9	23
62	Probing the effect of electron donation on CO2 absorbing 1,2,3-triazolide ionic liquids. RSC Advances, 2014, 4, 12748.	3.6	21
63	A density functional theory parameterised neural network model of zirconia. Molecular Simulation, 2018, 44, 623-630.	2.0	20
64	Relating the electronic structure and reactivity of the 3d transition metal monoxide surfaces. Catalysis Communications, 2014, 52, 60-64.	3.3	19
65	Effects of strain, d-band filling, and oxidation state on the bulk electronic structure of cubic 3d perovskites. Journal of Chemical Physics, 2011, 135, 104702.	3.0	18
66	Examples of Effective Data Sharing in Scientific Publishing. ACS Catalysis, 2015, 5, 3894-3899.	11.2	18
67	Correlation of Electronic Structure with Catalytic Activity: H₂â€“D₂ Exchange across Cu_xPd_{1â€“x} Composition Space. ACS Catalysis, 2015, 5, 3137-3147.	11.2	18
68	Open Challenges in Developing Generalizable Large-Scale Machine-Learning Models for Catalyst Discovery. ACS Catalysis, 2022, 12, 8572-8581.	11.2	18
69	H3PW12O40-functionalized tip for scanning tunneling microscopy. Proceedings of the National Academy of Sciences of the United States of America, 2002, 99, 6471-6475.	7.1	17
70	Simulating Temperature Programmed Desorption of Oxygen on Pt(111) Using DFT Derived Coverage Dependent Desorption Barriers. Topics in Catalysis, 2014, 57, 106-117.	2.8	17
71	Property prediction of crystalline solids from composition and crystal structure. AICHE Journal, 2016, 62, 2605-2613.	3.6	17
72	First-Principles Investigation of the Epitaxial Stabilization of Oxide Polymorphs: TiO₂ on (Sr,Ba)TiO₃. ACS Applied Materials & Interfaces, 2017, 9, 4106-4118.	8.0	17

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73	Modeling palladium surfaces with density functional theory, neural networks and molecular dynamics. Catalysis Today, 2018, 312, 132-140.	4.4	15
74	Acceleration of catalyst discovery with easy, fast, and reproducible computational alchemy. International Journal of Quantum Chemistry, 2021, 121, e26380.	2.0	15
75	A four-point probe correlation of oxygen sensitivity to changes in surface resistivity of TiO2(001) and Pd-modified TiO2(001). Surface Science, 2003, 545, L741-L746.	1.9	13
76	Highâ€throughput methods using composition and structure spread libraries. AICHE Journal, 2016, 62, 3826-3835.	3.6	13
77	First-principles study of the Cu-Pd phase diagram. Calphad: Computer Coupling of Phase Diagrams and Thermochemistry, 2017, 56, 224-229.	1.6	13
78	Core level shifts in Cuâ€“Pd alloys as a function of bulk composition and structure. Surface Science, 2015, 640, 127-132.	1.9	11
79	Comparative microfluidic screening of amino acid salt solutions for post-combustion CO2 capture. International Journal of Greenhouse Gas Control, 2015, 43, 189-197.	4.6	11
80	Semi-grand canonical Monte Carlo simulation of the acrolein induced surface segregation and aggregation of AgPd with machine learning surrogate models. Journal of Chemical Physics, 2021, 154, 134701.	3.0	11
81	Structure and Relative Thermal Stability of Mesoporous (<scp><scp>La</scp></scp>,<scp><scp>Sr</scp></scp>)<scp><scp>MnO₃</scp></scp> Powders Prepared Using Evaporationâ€Induced Selfâ€Assembly Methods. Journal of the American Ceramic Society, 2012, 95, 2339-2346.	3.8	9
82	Uncertainty quantification in machine learning and nonlinear least squares regression models. AICHE Journal, 2022, 68, e17516.	3.6	9
83	Sulphur poisoning of water-gas shift catalysts: site blocking and electronic structure modification. Molecular Simulation, 2009, 35, 936-941.	2.0	7
84	Preparation of Mesoporous La0.8Sr0.2MnO3 Infiltrated Coatings in Porous SOFC Cathodes Using Evaporation-Induced Self-Assembly Methods. ECS Transactions, 2011, 35, 2387-2399.	0.5	7
85	Coverage dependent adsorption properties of atomic adsorbates on late transition metal surfaces. Catalysis, 0, , 83-115.	1.0	7
86	Simulating Segregation in a Ternary Cuâ€“Pdâ€“Au Alloy with Density Functional Theory, Machine Learning, and Monte Carlo Simulations. Journal of Physical Chemistry C, 2022, 126, 1800-1808.	3.1	7
87	Accelerated optimization of pure metal and ligand compositions for light-driven hydrogen production. Reaction Chemistry and Engineering, 2022, 7, 599-608.	3.7	6
88	Ligand Enhanced Activity of In Situ Formed Nanoparticles for Photocatalytic Hydrogen Evolution. ChemCatChem, 2022, 14, .	3.7	6
89	The role of vdW interactions in coverage dependent adsorption energies of atomic adsorbates on Pt(111) and Pd(111). Surface Science, 2016, 650, 196-202.	1.9	5
90	Data sharing in Surface Science. Surface Science, 2016, 647, 103-107.	1.9	3

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91	Model-Specific to Model-General Uncertainty for Physical Properties. Industrial & Engineering Chemistry Research, 2022, 61, 8368-8377.	3.7	3
92	Automating data sharing through authoring tools. International Journal on Digital Libraries, 2017, 18, 93-98.	1.5	2
93	Evaluation of the degree of rate control via automatic differentiation. AIChE Journal, 2022, 68, .	3.6	1
94	Origin of the Stokesâ€“Einstein deviation in liquid Alâ€“Si. Molecular Simulation, 2022, 48, 303-313.	2.0	1
95	Rotational isomeric state theory applied to the stiffness prediction of an anion polymer electrolyte membrane. Proceedings of SPIE, 2008, , .	0.8	0
96	Preface: Trends in Computational Catalysis. Topics in Catalysis, 2012, 55, 227-228.	2.8	0