

John R Kitchin

List of Publications by Year in descending order

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96
papers

25,489
citations

81900

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39675

94
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105
docs citations

105
times ranked

22783
citing authors

#	ARTICLE	IF	CITATIONS
1	Uncertainty quantification in machine learning and nonlinear least squares regression models. <i>AIChE Journal</i> , 2022, 68, e17516.	3.6	9
2	Accelerated optimization of pure metal and ligand compositions for light-driven hydrogen production. <i>Reaction Chemistry and Engineering</i> , 2022, 7, 599-608.	3.7	6
3	Ligand Enhanced Activity of In Situ Formed Nanoparticles for Photocatalytic Hydrogen Evolution. <i>ChemCatChem</i> , 2022, 14, .	3.7	6
4	Simulating Segregation in a Ternary Cu-Pd-Au Alloy with Density Functional Theory, Machine Learning, and Monte Carlo Simulations. <i>Journal of Physical Chemistry C</i> , 2022, 126, 1800-1808.	3.1	7
5	Model-Specific to Model-General Uncertainty for Physical Properties. <i>Industrial & Engineering Chemistry Research</i> , 2022, 61, 8368-8377.	3.7	3
6	Evaluation of the degree of rate control via automatic differentiation. <i>AIChE Journal</i> , 2022, 68, .	3.6	1
7	Origin of the Stokes-Einstein deviation in liquid Al-Si. <i>Molecular Simulation</i> , 2022, 48, 303-313.	2.0	1
8	Open Challenges in Developing Generalizable Large-Scale Machine-Learning Models for Catalyst Discovery. <i>ACS Catalysis</i> , 2022, 12, 8572-8581.	11.2	18
9	Acceleration of catalyst discovery with easy, fast, and reproducible computational alchemy. <i>International Journal of Quantum Chemistry</i> , 2021, 121, e26380.	2.0	15
10	Semi-grand canonical Monte Carlo simulation of the acrolein induced surface segregation and aggregation of AgPd with machine learning surrogate models. <i>Journal of Chemical Physics</i> , 2021, 154, 134701.	3.0	11
11	Machine-learning accelerated geometry optimization in molecular simulation. <i>Journal of Chemical Physics</i> , 2021, 154, 234704.	3.0	27
12	SingleNN: Modified Behler-Parrinello Neural Network with Shared Weights for Atomistic Simulations with Transferability. <i>Journal of Physical Chemistry C</i> , 2020, 124, 17811-17818.	3.1	26
13	Parallelized Screening of Characterized and DFT-Modeled Bimetallic Colloidal Cocatalysts for Photocatalytic Hydrogen Evolution. <i>ACS Catalysis</i> , 2020, 10, 4244-4252.	11.2	41
14	pybliometrics: Scriptable bibliometrics using a Python interface to Scopus. <i>SoftwareX</i> , 2019, 10, 100263.	2.6	96
15	Machine learning in catalysis. <i>Nature Catalysis</i> , 2018, 1, 230-232.	34.4	308
16	Investigating the Reactivity of Single Atom Alloys Using Density Functional Theory. <i>Topics in Catalysis</i> , 2018, 61, 462-474.	2.8	117
17	A density functional theory parameterised neural network model of zirconia. <i>Molecular Simulation</i> , 2018, 44, 623-630.	2.0	20
18	Modeling palladium surfaces with density functional theory, neural networks and molecular dynamics. <i>Catalysis Today</i> , 2018, 312, 132-140.	4.4	15

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19	Modeling Segregation on AuPd(111) Surfaces with Density Functional Theory and Monte Carlo Simulations. <i>Journal of Physical Chemistry C</i> , 2017, 121, 3479-3487.	3.1	48
20	Neural network predictions of oxygen interactions on a dynamic Pd surface. <i>Molecular Simulation</i> , 2017, 43, 346-354.	2.0	58
21	First-principles study of the Cu-Pd phase diagram. <i>Calphad: Computer Coupling of Phase Diagrams and Thermochemistry</i> , 2017, 56, 224-229.	1.6	13
22	The atomic simulation environmentâ€”a Python library for working with atoms. <i>Journal of Physics Condensed Matter</i> , 2017, 29, 273002.	1.8	1,933
23	First-Principles Investigation of the Epitaxial Stabilization of Oxide Polymorphs: TiO ₂ on (Sr,Ba)TiO ₃ . <i>ACS Applied Materials & Interfaces</i> , 2017, 9, 4106-4118.	8.0	17
24	Alchemical Predictions for Computational Catalysis: Potential and Limitations. <i>Journal of Physical Chemistry Letters</i> , 2017, 8, 5002-5007.	4.6	48
25	Automating data sharing through authoring tools. <i>International Journal on Digital Libraries</i> , 2017, 18, 93-98.	1.5	2
26	Competitive Growth of Scrutinyite (Î±-PbO ₂) and Rutile Polymorphs of SnO ₂ on All Orientations of Columbite CoNb ₂ O ₆ Substrates. <i>Crystal Growth and Design</i> , 2017, 17, 3929-3939.	3.0	25
27	Neural network and ReaxFF comparison for Au properties. <i>International Journal of Quantum Chemistry</i> , 2016, 116, 979-987.	2.0	66
28	Quantifying Uncertainty in Activity Volcano Relationships for Oxygen Reduction Reaction. <i>ACS Catalysis</i> , 2016, 6, 5251-5259.	11.2	70
29	High-throughput methods using composition and structure spread libraries. <i>AIChE Journal</i> , 2016, 62, 3826-3835.	3.6	13
30	The role of vdW interactions in coverage dependent adsorption energies of atomic adsorbates on Pt(111) and Pd(111). <i>Surface Science</i> , 2016, 650, 196-202.	1.9	5
31	Property prediction of crystalline solids from composition and crystal structure. <i>AIChE Journal</i> , 2016, 62, 2605-2613.	3.6	17
32	Data sharing in Surface Science. <i>Surface Science</i> , 2016, 647, 103-107.	1.9	3
33	Toward Benchmarking in Catalysis Science: Best Practices, Challenges, and Opportunities. <i>ACS Catalysis</i> , 2016, 6, 2590-2602.	11.2	190
34	Examples of Effective Data Sharing in Scientific Publishing. <i>ACS Catalysis</i> , 2015, 5, 3894-3899.	11.2	18
35	Redox-Mediated Separation of Carbon Dioxide from Flue Gas. <i>Energy & Fuels</i> , 2015, 29, 7508-7515.	5.1	48
36	Investigating the Energetic Ordering of Stable and Metastable TiO ₂ Polymorphs Using DFT+ <i>U</i> and Hybrid Functionals. <i>Journal of Physical Chemistry C</i> , 2015, 119, 21060-21071.	3.1	81

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37	A Linear Response DFT+ <i>U</i> Study of Trends in the Oxygen Evolution Activity of Transition Metal Rutile Dioxides. <i>Journal of Physical Chemistry C</i> , 2015, 119, 4827-4833.	3.1	86
38	Estimating Bulk-Composition-Dependent H ₂ Adsorption Energies on Cu _x Pd _{1-x} Alloy (111) Surfaces. <i>ACS Catalysis</i> , 2015, 5, 1020-1026.	11.2	24
39	Core level shifts in CuPd alloys as a function of bulk composition and structure. <i>Surface Science</i> , 2015, 640, 127-132.	1.9	11
40	Relationships between the surface electronic and chemical properties of doped 4d and 5d late transition metal dioxides. <i>Journal of Chemical Physics</i> , 2015, 142, 104703.	3.0	28
41	Alkaline Electrolyte and Fe Impurity Effects on the Performance and Active-Phase Structure of NiOOH Thin Films for OER Catalysis Applications. <i>Journal of Physical Chemistry C</i> , 2015, 119, 11475-11481.	3.1	110
42	Correlation of Electronic Structure with Catalytic Activity: H ₂ D ₂ Exchange across Cu _x Pd _{1-x} Composition Space. <i>ACS Catalysis</i> , 2015, 5, 3137-3147.	11.2	18
43	Accurate electronic and chemical properties of 3d transition metal oxides using a calculated linear response <i>U</i> and a DFT + <i>U</i> (V) method. <i>Journal of Chemical Physics</i> , 2015, 142, 144701.	3.0	27
44	Comparative microfluidic screening of amino acid salt solutions for post-combustion CO ₂ capture. <i>International Journal of Greenhouse Gas Control</i> , 2015, 43, 189-197.	4.6	11
45	Tuning oxide activity through modification of the crystal and electronic structure: from strain to potential polymorphs. <i>Physical Chemistry Chemical Physics</i> , 2015, 17, 28943-28949.	2.8	31
46	Effects of Concentration, Crystal Structure, Magnetism, and Electronic Structure Method on First-Principles Oxygen Vacancy Formation Energy Trends in Perovskites. <i>Journal of Physical Chemistry C</i> , 2014, 118, 28776-28790.	3.1	105
47	Probing the Coverage Dependence of Site and Adsorbate Configurational Correlations on (111) Surfaces of Late Transition Metals. <i>Journal of Physical Chemistry C</i> , 2014, 118, 25597-25602.	3.1	29
48	Probing the effect of electron donation on CO ₂ absorbing 1,2,3-triazolide ionic liquids. <i>RSC Advances</i> , 2014, 4, 12748.	3.6	21
49	Electrocatalytic Oxygen Evolution with an Immobilized TAML Activator. <i>Journal of the American Chemical Society</i> , 2014, 136, 5603-5606.	13.7	71
50	Identifying Potential BO ₂ Oxide Polymorphs for Epitaxial Growth Candidates. <i>ACS Applied Materials & Interfaces</i> , 2014, 6, 3630-3639.	8.0	26
51	Simulating Temperature Programmed Desorption of Oxygen on Pt(111) Using DFT Derived Coverage Dependent Desorption Barriers. <i>Topics in Catalysis</i> , 2014, 57, 106-117.	2.8	17
52	Relating the electronic structure and reactivity of the 3d transition metal monoxide surfaces. <i>Catalysis Communications</i> , 2014, 52, 60-64.	3.3	19
53	Comparisons of amine solvents for post-combustion CO ₂ capture: A multi-objective analysis approach. <i>International Journal of Greenhouse Gas Control</i> , 2013, 18, 68-74.	4.6	46
54	Number of outer electrons as descriptor for adsorption processes on transition metals and their oxides. <i>Chemical Science</i> , 2013, 4, 1245.	7.4	273

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55	Interactions in 1-ethyl-3-methyl imidazolium tetracyanoborate ion pair: Spectroscopic and density functional study. <i>Journal of Molecular Structure</i> , 2013, 1038, 12-18.	3.6	31
56	Effects of O ₂ and SO ₂ on the Capture Capacity of a Primary-Amine Based Polymeric CO ₂ Sorbent. <i>Industrial & Engineering Chemistry Research</i> , 2013, 52, 10788-10794.	3.7	68
57	Chemical and Molecular Descriptors for the Reactivity of Amines with CO ₂ . <i>Industrial & Engineering Chemistry Research</i> , 2012, 51, 13609-13618.	3.7	24
58	Evaluation of a Primary Amine-Functionalized Ion-Exchange Resin for CO ₂ Capture. <i>Industrial & Engineering Chemistry Research</i> , 2012, 51, 6907-6915.	3.7	97
59	The outlook for improved carbon capture technology. <i>Progress in Energy and Combustion Science</i> , 2012, 38, 630-671.	31.2	427
60	Effects of strain, <i>d</i> -band filling, and oxidation state on the surface electronic structure and reactivity of 3 <i>d</i> perovskite surfaces. <i>Journal of Chemical Physics</i> , 2012, 137, 084703.	3.0	67
61	Spectroscopic Characterization of Mixed Fe-Ni Oxide Electrocatalysts for the Oxygen Evolution Reaction in Alkaline Electrolytes. <i>ACS Catalysis</i> , 2012, 2, 1793-1801.	11.2	423
62	Preface: Trends in Computational Catalysis. <i>Topics in Catalysis</i> , 2012, 55, 227-228.	2.8	0
63	Structure and Relative Thermal Stability of Mesoporous (La, Sr)MnO ₃ Powders Prepared Using Evaporation-Induced Self-Assembly Methods. <i>Journal of the American Ceramic Society</i> , 2012, 95, 2339-2346.	3.8	9
64	Identification of Sulfur-Tolerant Bimetallic Surfaces Using DFT Parametrized Models and Atomistic Thermodynamics. <i>ACS Catalysis</i> , 2011, 1, 399-407.	11.2	24
65	Effects of strain, <i>d</i> -band filling, and oxidation state on the bulk electronic structure of cubic 3 <i>d</i> perovskites. <i>Journal of Chemical Physics</i> , 2011, 135, 104702.	3.0	18
66	Universality in Oxygen Evolution Electrocatalysis on Oxide Surfaces. <i>ChemCatChem</i> , 2011, 3, 1159-1165.	3.7	3,208
67	Configurational correlations in the coverage dependent adsorption energies of oxygen atoms on late transition metal fcc(111) surfaces. <i>Journal of Chemical Physics</i> , 2011, 134, 104709.	3.0	58
68	Preparation of Mesoporous La _{0.8} Sr _{0.2} MnO ₃ Infiltrated Coatings in Porous SOFC Cathodes Using Evaporation-Induced Self-Assembly Methods. <i>ECS Transactions</i> , 2011, 35, 2387-2399.	0.5	7
69	CO ₂ Adsorption on Supported Molecular Amidine Systems on Activated Carbon. <i>ChemSusChem</i> , 2010, 3, 948-956.	6.8	32
70	Separation of CO ₂ from flue gas using electrochemical cells. <i>Fuel</i> , 2010, 89, 1307-1314.	6.4	52
71	Simple model explaining and predicting coverage-dependent atomic adsorption energies on transition metal surfaces. <i>Physical Review B</i> , 2010, 82, .	3.2	62
72	New solid-state table: estimating d-band characteristics for transition metal atoms. <i>Molecular Simulation</i> , 2010, 36, 633-638.	2.0	37

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73	Electrochemical Concentration of Carbon Dioxide from an Oxygen/Carbon Dioxide Containing Gas Stream. Journal of the Electrochemical Society, 2010, 157, B1149.	2.9	23
74	Correlations in coverage-dependent atomic adsorption energies on Pd(111). Physical Review B, 2009, 79, .	3.2	87
75	Sulphur poisoning of water-gas shift catalysts: site blocking and electronic structure modification. Molecular Simulation, 2009, 35, 936-941.	2.0	7
76	Step decoration of chiral metal surfaces. Journal of Chemical Physics, 2009, 130, 124710.	3.0	27
77	Atomistic thermodynamics study of the adsorption and the effects of water-gas shift reactants on Cu catalysts under reaction conditions. Journal of Catalysis, 2009, 261, 188-194.	6.2	41
78	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
79	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
80	Hydrogen Dissociation and Spillover on Individual Isolated Palladium Atoms. Physical Review Letters, 2009, 103, 246102.	7.8	216
81	Alloy surface segregation in reactive environments: First-principles atomistic thermodynamics study of Ag_3Pd oxygen atmospheres. Physical Review B, 2008, 77, .	3.2	129
82	Rotational isomeric state theory applied to the stiffness prediction of an anion polymer electrolyte membrane. Proceedings of SPIE, 2008, , .	0.8	0
83	Response to "Comment on "Trends in the Exchange Current for Hydrogen Evolution" [J. Electrochem. Soc., 152, J23 (2005)]". Journal of the Electrochemical Society, 2006, 153, L33.	2.9	29
84	Trends in the chemical properties of early transition metal carbide surfaces: A density functional study. Catalysis Today, 2005, 105, 66-73.	4.4	302
85	Trends in the Exchange Current for Hydrogen Evolution. Journal of the Electrochemical Society, 2005, 152, J23.	2.9	4,054
86	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
87	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
88	The Role of Adsorbate-Adsorbate Interactions in the Rate Controlling Step and the Most Abundant Reaction Intermediate of NH_3 Decomposition on Ru. Catalysis Letters, 2004, 96, 13-22.	2.6	76
89	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
90	A four-point probe correlation of oxygen sensitivity to changes in surface resistivity of $\text{TiO}_2(001)$ and Pd-modified $\text{TiO}_2(001)$. Surface Science, 2003, 545, L741-L746.	1.9	13

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91	Elucidation of the active surface and origin of the weak metal-hydrogen bond on Ni/Pt(111) bimetallic surfaces: a surface science and density functional theory study. <i>Surface Science</i> , 2003, 544, 295-308.	1.9	154
92	A comparison of gold and molybdenum nanoparticles on TiO ₂ (100) reconstructed single crystal surfaces. <i>Surface Science</i> , 2003, 526, 323-331.	1.9	38
93	H ₃ PW ₁₂ O ₄₀ -functionalized tip for scanning tunneling microscopy. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2002, 99, 6471-6475.	7.1	17
94	Preparation of Paramagnetic Ligands for Coordination-Complexes and Networks with Interesting Magnetic Properties. <i>Molecular Crystals and Liquid Crystals</i> , 1997, 305, 303-310.	0.3	25
95	Preparation and Characterization of a Bis-Semiquinone: a Bidentate Dianion Biradical. <i>Journal of Organic Chemistry</i> , 1995, 60, 3578-3579.	3.2	34
96	Coverage dependent adsorption properties of atomic adsorbates on late transition metal surfaces. <i>Catalysis</i> , 0, , 83-115.	1.0	7