Heather J Kulik

List of Publications by Year
in descending order

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125 papers	6,168 citations	71061 41 h-index	79644 73 g-index
168 all docs	168 docs citations	168 times ranked	6004 citing authors

#	Article	IF	Citations
1	Density Functional Theory in Transition-Metal Chemistry: A Self-Consistent HubbardUApproach. Physical Review Letters, 2006, 97, 103001.	2.9	526
2	Understanding the diversity of the metal-organic framework ecosystem. Nature Communications, 2020, 11, 4068.	5.8	282
3	Protection of tissue physicochemical properties using polyfunctional crosslinkers. Nature Biotechnology, 2019, 37, 73-83.	9.4	262
4	Critical Knowledge Gaps in Mass Transport through Single-Digit Nanopores: A Review and Perspective. Journal of Physical Chemistry C, 2019, 123, 21309-21326.	1.5	234
5	Mechanically triggered heterolytic unzipping of a low-ceiling-temperature polymer. Nature Chemistry, 2014, 6, 623-628.	6.6	198
6	Resolving Transition Metal Chemical Space: Feature Selection for Machine Learning and Structureâ€“Property Relationships. Journal of Physical Chemistry A, 2017, 121, 8939-8954.	1.1	168
7	Perspective: Treating electron over-delocalization with the DFT+U method. Journal of Chemical Physics, 2015, 142, 240901.	1.2	154
8	Predicting electronic structure properties of transition metal complexes with neural networks. Chemical Science, 2017, 8, 5137-5152.	3.7	152
9	How Large Should the QM Region Be in QM/MM Calculations? The Case of Catechol O-Methyltransferase. Journal of Physical Chemistry B, 2016, 120, 11381-11394.	1.2	150
10	Accelerating Chemical Discovery with Machine Learning: Simulated Evolution of Spin Crossover Complexes with an Artificial Neural Network. Journal of Physical Chemistry Letters, 2018, 9, 1064-1071.	2.1	145
11	A quantitative uncertainty metric controls error in neural network-driven chemical discovery. Chemical Science, 2019, 10, 7913-7922.	3.7	129
12	molSimplify: A toolkit for automating discovery in inorganic chemistry. Journal of Computational Chemistry, 2016, 37, 2106-2117.	1.5	127
13	Understanding and Breaking Scaling Relations in Single-Site Catalysis: Methane to Methanol Conversion by Fe^{IV}â•O. ACS Catalysis, 2018, 8, 975-986.	5.5	119
14	Accurate Multiobjective Design in a Space of Millions of Transition Metal Complexes with Neural-Network-Driven Efficient Global Optimization. ACS Central Science, 2020, 6, 513-524.	5.3	114
15	Computational Discovery of Transition-metal Complexes: From High-throughput Screening to Machine Learning. Chemical Reviews, 2021, 121, 9927-10000.	23.0	110
16	Anionâ€Selective Redox Electrodes: Electrochemically Mediated Separation with Heterogeneous Organometallic Interfaces. Advanced Functional Materials, 2016, 26, 3394-3404.	7.8	106
17	Strategies and Software for Machine Learning Accelerated Discovery in Transition Metal Chemistry. Industrial & Engineering Chemistry Research, 2018, 57, 13973-13986.	1.8	104
18	Ab Initio Quantum Chemistry for Protein Structures. Journal of Physical Chemistry B, 2012, 116, 12501-12509.	1.2	99

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19	Towards quantifying the role of exact exchange in predictions of transition metal complex properties. Journal of Chemical Physics, 2015, 143, 034104.	1.2	93
20	Quantum Chemistry for Solvated Molecules on Graphical Processing Units Using Polarizable Continuum Models. Journal of Chemical Theory and Computation, 2015, 11, 3131-3144.	2.3	91
21	Systematic study of first-row transition-metal diatomic molecules: A self-consistent DFT+U approach. Journal of Chemical Physics, 2010, 133, 114103.	1.2	87
22	Ionization behavior of nanoporous polyamide membranes. Proceedings of the National Academy of Sciences of the United States of America, 2020, 117, 30191-30200.	3.3	82
23	Designing in the Face of Uncertainty: Exploiting Electronic Structure and Machine Learning Models for Discovery in Inorganic Chemistry. Inorganic Chemistry, 2019, 58, 10592-10606.	1.9	79
24	A self-consistent Hubbard U density-functional theory approach to the addition-elimination reactions of hydrocarbons on bare FeO+. Journal of Chemical Physics, 2008, 129, 134314.	1.2	72
25	Systematic Quantum Mechanical Region Determination in QM/MM Simulation. Journal of Chemical Theory and Computation, 2017, 13, 563-576.	2.3	72
26	Using Machine Learning and Data Mining to Leverage Community Knowledge for the Engineering of Stable Metalâ€“Organic Frameworks. Journal of the American Chemical Society, 2021, 143, 17535-17547.	6.6	71
27	Machine Learning Accelerates the Discovery of Design Rules and Exceptions in Stable Metalâ€“Oxo Intermediate Formation. ACS Catalysis, 2019, 9, 8243-8255.	5.5	67
28	Learning from Failure: Predicting Electronic Structure Calculation Outcomes with Machine Learning Models. Journal of Chemical Theory and Computation, 2019, 15, 2331-2345.	2.3	66
29	Mediation of donorâ€“acceptor distance in an enzymatic methyl transfer reaction. Proceedings of the National Academy of Sciences of the United States of America, 2015, 112, 7954-7959.	3.3	65
30	Where Does the Density Localize? Convergent Behavior for Global Hybrids, Range Separation, and DFT+U. Journal of Chemical Theory and Computation, 2016, 12, 5931-5945.	2.3	65
31	Accurate potential energy surfaces with a DFT+$U(mathbf {R})$U(R) approach. Journal of Chemical Physics, 2011, 135, 194105.	1.2	63
32	Where Does the Density Localize in the Solid State? Divergent Behavior for Hybrids and DFT+U. Journal of Chemical Theory and Computation, 2018, 14, 670-683.	2.3	57
33	Transition-metal dioxides: A case for the intersite term in Hubbard-model functionals. Journal of Chemical Physics, 2011, 134, 094103.	1.2	55
34	Ligand-Field-Dependent Behavior of Meta-GGA Exchange in Transition-Metal Complex Spin-State Ordering. Journal of Physical Chemistry A, 2017, 121, 874-884.	1.1	52
35	Substrate Placement Influences Reactivity in Non-heme Fe(II) Halogenases and Hydroxylases. Journal of Biological Chemistry, 2013, 288, 11233-11241.	1.6	51
36	First-Principles Study of Non-heme Fe(II) Halogenase SyrB2 Reactivity. Journal of the American Chemical Society, 2009, 131, 14426-14433.	6.6	50

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37	Seeing Is Believing: Experimental Spin States from Machine Learning Model Structure Predictions. Journal of Physical Chemistry A, 2020, 124, 3286-3299.	1.1	48
38	Leveraging Cheminformatics Strategies for Inorganic Discovery: Application to Redox Potential Design. Industrial & Engineering Chemistry Research, 2017, 56, 4898-4910.	1.8	45
39	Machine learning reveals key ion selectivity mechanisms in polymeric membranes with subnanometer pores. Science Advances, 2022, 8, eabl5771.	4.7	45
40	Probing the Structure of Salt Water under Confinement with First-Principles Molecular Dynamics and Theoretical X-ray Absorption Spectroscopy. Journal of Physical Chemistry Letters, 2012, 3, 2653-2658.	2.1	43
41	Unifying Exchange Sensitivity in Transition-Metal Spin-State Ordering and Catalysis through Bond Valence Metrics. Journal of Chemical Theory and Computation, 2017, 13, 5443-5457.	2.3	43
42	Harder, better, faster, stronger: Large-scale QM and QM/MM for predictive modeling in enzymes and proteins. Current Opinion in Structural Biology, 2022, 72, 9-17.	2.6	42
43	Irreversible synthesis of an ultrastrong two-dimensional polymeric material. Nature, 2022, 602, 91-95.	13.7	42
44	Local Effects in the X-ray Absorption Spectrum of Salt Water. Journal of Physical Chemistry B, 2010, 114, 9594-9601.	1.2	41
45	Rapid Detection of Strong Correlation with Machine Learning for Transition-Metal Complex High-Throughput Screening. Journal of Physical Chemistry Letters, 2020, 11, 8067-8076.	2.1	40
46	Density functional theory for modelling large molecular adsorbateâ€“surface interactions: a mini-review and worked example. Molecular Simulation, 2017, 43, 327-345.	0.9	39
47	Large-scale QM/MM free energy simulations of enzyme catalysis reveal the influence of charge transfer. Physical Chemistry Chemical Physics, 2018, 20, 20650-20660.	1.3	39
48	Global and local curvature in density functional theory. Journal of Chemical Physics, 2016, 145, 054109.	1.2	38
49	Evaluating Unexpectedly Short Non-covalent Distances in X-ray Crystal Structures of Proteins with Electronic Structure Analysis. Journal of Chemical Information and Modeling, 2019, 59, 2199-2211.	2.5	38
50	Computational Investigation of the Interplay of Substrate Positioning and Reactivity in Catechol O-Methyltransferase. PLoS ONE, 2016, 11, e0161868.	1.1	36
51	Communication: Recovering the flat-plane condition in electronic structure theory at semi-local DFT cost. Journal of Chemical Physics, 2017, 147, 191101.	1.2	34
52	Bridging the Homogeneous-Heterogeneous Divide: Modeling Spin for Reactivity in Single Atom Catalysis. Frontiers in Chemistry, 2019, 7, 219.	1.8	34
53	Exploiting graphical processing units to enable quantum chemistry calculation of large solvated molecules with conductorâ€like polarizable continuum models. International Journal of Quantum Chemistry, 2019, 119, e25760.	1.0	34
54	Making machine learning a useful tool in the accelerated discovery of transition metal complexes. Wiley Interdisciplinary Reviews: Computational Molecular Science, 2020, 10, e1439.	6.2	34

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55	Navigating Transition-Metal Chemical Space: Artificial Intelligence for First-Principles Design. Accounts of Chemical Research, 2021, 54, 532-545.	7.6	34
56	MOFSimplify, machine learning models with extracted stability data of three thousand metalâ€“organic frameworks. Scientific Data, 2022, 9, 74.	2.4	34
57	Revealing quantum mechanical effects in enzyme catalysis with large-scale electronic structure simulation. Reaction Chemistry and Engineering, 2019, 4, 298-315.	1.9	33
58	Why Conventional Design Rules for Câ€“H Activation Fail for Open-Shell Transition-Metal Catalysts. ACS Catalysis, 2020, 10, 15033-15047.	5.5	30
59	The Proteinâ€™s Role in Substrate Positioning and Reactivity for Biosynthetic Enzyme Complexes: The Case of SyrB2/SyrB1. ACS Catalysis, 2019, 9, 4930-4943.	5.5	28
60	Data-Driven Approaches Can Overcome the Costâ€“Accuracy Trade-Off in Multireference Diagnostics. Journal of Chemical Theory and Computation, 2020, 16, 4373-4387.	2.3	28
61	Both Configuration and QM Region Size Matter: Zinc Stability in QM/MM Models of DNA Methyltransferase. Journal of Chemical Theory and Computation, 2020, 16, 3121-3134.	2.3	28
62	Putting Density Functional Theory to the Test in Machine-Learning-Accelerated Materials Discovery. Journal of Physical Chemistry Letters, 2021, 12, 4628-4637.	2.1	28
63	Stable Surfaces That Bind Too Tightly: Can Range-Separated Hybrids or DFT+U Improve Paradoxical Descriptions of Surface Chemistry?. Journal of Physical Chemistry Letters, 2019, 10, 5090-5098.	2.1	27
64	Semi-supervised Machine Learning Enables the Robust Detection of Multireference Character at Low Cost. Journal of Physical Chemistry Letters, 2020, 11, 6640-6648.	2.1	27
65	Anthracene as a Launchpad for a Phosphinidene Sulfide and for Generation of a Phosphorusâ€“Sulfur Material Having the Composition P₂S, a Vulcanized Red Phosphorus That Is Yellow. Journal of the American Chemical Society, 2019, 141, 431-440.	6.6	26
66	Electronic Structure Origins of Surface-Dependent Growth in IIIâ€“V Quantum Dots. Chemistry of Materials, 2018, 30, 7154-7165.	3.2	25
67	Harnessing Organic Ligand Libraries for First-Principles Inorganic Discovery: Indium Phosphide Quantum Dot Precursor Design Strategies. Chemistry of Materials, 2017, 29, 3632-3643.	3.2	24
68	Endohedrally Functionalized Metalâ€“Organic Cage-Cross-Linked Polymer Gels as Modular Heterogeneous Catalysts. Journal of the American Chemical Society, 2022, 144, 13276-13284.	6.6	24
69	Enumeration of de novo inorganic complexes for chemical discovery and machine learning. Molecular Systems Design and Engineering, 2020, 5, 139-152.	1.7	23
70	Machine learning to tame divergent density functional approximations: a new path to consensus materials design principles. Chemical Science, 2021, 12, 13021-13036.	3.7	23
71	New Strategies for Direct Methane-to-Methanol Conversion from Active Learning Exploration of 16 Million Catalysts. Jacs Au, 2022, 2, 1200-1213.	3.6	23
72	Impact of Approximate DFT Density Delocalization Error on Potential Energy Surfaces in Transition Metal Chemistry. Journal of Chemical Theory and Computation, 2020, 16, 264-277.	2.3	22

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73	Quantum Mechanical Description of Electrostatics Provides a Unified Picture of Catalytic Action Across Methyltransferases. Journal of Physical Chemistry Letters, 2019, 10, 3779-3787.	2.1	21
74	Audacity of huge: overcoming challenges of data scarcity and data quality for machine learning in computational materials discovery. Current Opinion in Chemical Engineering, 2022, 36, 100778.	3.8	21
75	Direct Observation of Early-Stage Quantum Dot Growth Mechanisms with High-Temperature Ab Initio Molecular Dynamics. Journal of Physical Chemistry C, 2016, 120, 2472-2483.	1.5	20
76	Depolymerization Pathways for Branching Lignin Spirodienone Units Revealed with ab Initio Steered Molecular Dynamics. Journal of Physical Chemistry A, 2017, 121, 532-543.	1.1	20
77	Large-scale comparison of 3d and 4d transition metal complexes illuminates the reduced effect of exchange on second-row spin-state energetics. Physical Chemistry Chemical Physics, 2020, 22, 19326-19341.	1.3	20
78	Spectroscopically Guided Simulations Reveal Distinct Strategies for Positioning Substrates to Achieve Selectivity in Nonheme Fe(II)/Î±-Ketoglutarate-Dependent Halogenases. ACS Catalysis, 2021, 11, 12394-12408.	5.5	20
79	Adapting DFT+U for the Chemically Motivated Correction of Minimal Basis Set Incompleteness. Journal of Physical Chemistry A, 2016, 120, 5939-5949.	1.1	19
80	Designing small-molecule catalysts for CO2 capture. Energy Procedia, 2011, 4, 817-823.	1.8	18
81	Advancing Discovery in Chemistry with Artificial Intelligence: From Reaction Outcomes to New Materials and Catalysts. Accounts of Chemical Research, 2021, 54, 2335-2336.	7.6	18
82	Computational Discovery of Hydrogen Bond Design Rules for Electrochemical Ion Separation. Chemistry of Materials, 2016, 28, 6207-6218.	3.2	17
83	When are two hydrogen bonds better than one? Accurate first-principles models explain the balance of hydrogen bond donors and acceptors found in proteins. Chemical Science, 2021, 12, 1147-1162.	3.7	17
84	Ab Initio Screening Approach for the Discovery of Lignin Polymer Breaking Pathways. Journal of Physical Chemistry A, 2015, 119, 6551-6562.	1.1	16
85	Biochemical and crystallographic investigations into isonitrile formation by a nonheme iron-dependent oxidase/decarboxylase. Journal of Biological Chemistry, 2021, 296, 100231.	1.6	16
86	Quantum Chemistry Common Driver and Databases (QCDB) and Quantum Chemistry Engine (QCE<scp>ngine</scp>): Automation and interoperability among computational chemistry programs. Journal of Chemical Physics, 2021, 155, 204801.	1.2	15
87	Using Computational Chemistry To Reveal Natureâ€™s Blueprints for Single-Site Catalysis of Câ€“H Activation. ACS Catalysis, 2022, 12, 9281-9306.	5.5	15
88	Non-empirical, low-cost recovery of exact conditions with model-Hamiltonian inspired expressions in jmDFT. Journal of Chemical Physics, 2019, 150, 154115.	1.2	13
89	Developing an approach for first-principles catalyst design: application to carbon-capture catalysis. Acta Crystallographica Section C, Structural Chemistry, 2014, 70, 123-131.	0.2	12
90	Discovering Amorphous Indium Phosphide Nanostructures with High-Temperature ab Initio Molecular Dynamics. Journal of Physical Chemistry C, 2015, 119, 23238-23249.	1.5	12

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91	When Is Ligand pK_a a Good Descriptor for Catalyst Energetics? In Search of Optimal CO₂ Hydration Catalysts. Journal of Physical Chemistry A, 2018, 122, 4579-4590.	1.1	12
92	Modeling the roles of rigidity and dopants in single-atom methane-to-methanol catalysts. Journal of Materials Chemistry A, 2022, 10, 6193-6203.	5.2	12
93	The Effect of Hartree-Fock Exchange on Scaling Relations and Reaction Energetics for Câ€“H Activation Catalysts. Topics in Catalysis, 2022, 65, 296-311.	1.3	11
94	Molecular basis of C-S bond cleavage in the glycyl radical enzyme isethionate sulfite-lyase. Cell Chemical Biology, 2021, 28, 1333-1346.e7.	2.5	11
95	Representations and strategies for transferable machine learning improve model performance in chemical discovery. Journal of Chemical Physics, 2022, 156, 074101.	1.2	11
96	Machine Learning for the Discovery, Design, and Engineering of Materials. Annual Review of Chemical and Biomolecular Engineering, 2022, 13, 405-429.	3.3	10
97	Ab initio investigation of high multiplicity optical transitions in the spectra of CN and isoelectronic species. Journal of Molecular Spectroscopy, 2009, 258, 6-12.	0.4	9
98	Molecular DFT+U: A Transferable, Low-Cost Approach to Eliminate Delocalization Error. Journal of Physical Chemistry Letters, 2021, 12, 3633-3640.	2.1	9
99	Detection of multi-reference character imbalances enables a transfer learning approach for virtual high throughput screening with coupled cluster accuracy at DFT cost. Chemical Science, 2022, 13, 4962-4971.	3.7	9
100	Probing the Mechanism of Isonitrile Formation by a Non-Heme Iron(II)-Dependent Oxidase/Decarboxylase. Journal of the American Chemical Society, 2022, 144, 5893-5901.	6.6	9
101	Machine Learning Models Predict Calculation Outcomes with the Transferability Necessary for Computational Catalysis. Journal of Chemical Theory and Computation, 2022, 18, 4282-4292.	2.3	9
102	Influence of the Greater Protein Environment on the Electrostatic Potential in Metalloenzyme Active Sites: The Case of Formate Dehydrogenase. Journal of Physical Chemistry B, 2022, 126, 4069-4079.	1.2	8
103	Predicting the Stability of Fullerene Allotropes Throughout the Periodic Table. Journal of Physical Chemistry C, 2016, 120, 17035-17045.	1.5	7
104	Eliminating Delocalization Error to Improve Heterogeneous Catalysis Predictions with Molecular DFT + U. Journal of Chemical Theory and Computation, 2022, 18, 1142-1155.	2.3	7
105	Uncovering Alternate Pathways to Nafion Membrane Degradation in Fuel Cells with First-Principles Modeling. Journal of Physical Chemistry C, 2020, 124, 15094-15106.	1.5	6
106	What's Left for a Computational Chemist To Do in the Age of Machine Learning?. Israel Journal of Chemistry, 2022, 62, .	1.0	6
107	Mapping the Origins of Surface- and Chemistry-Dependent Doping Trends in IIIâ€“V Quantum Dots with Density Functional Theory. Chemistry of Materials, 2021, 33, 7113-7123.	3.2	6
108	Large-Scale Screening Reveals That Geometric Structure Matters More Than Electronic Structure in the Bioinspired Catalyst Design of Formate Dehydrogenase Mimics. ACS Catalysis, 2022, 12, 383-396.	5.5	5

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109	Are Vanadium Intermediates Suitable Mimics in Non-Heme Iron Enzymes? An Electronic Structure Analysis. ACS Catalysis, 2022, 12, 5489-5501.	5.5	5
110	Understanding the chemical bonding of ground and excited states of HfO and HfB with correlated wavefunction theory and density functional approximations. Journal of Chemical Physics, 2022, 156, 184113.	1.2	5
111	Coding solvation: challenges and opportunities. International Journal of Quantum Chemistry, 2019, 119, e25839.	1.0	4
112	Deciphering Cryptic Behavior in Bimetallic Transition-Metal Complexes with Machine Learning. Journal of Physical Chemistry Letters, 2021, 12, 9812-9820.	2.1	4
113	Computational Modeling of Conformer Stability in Benenodin-1, a Thermally Actuated Lasso Peptide Switch. Journal of Physical Chemistry B, 2022, 126, 3398-3406.	1.2	4
114	Exploiting Ligand Additivity for Transferable Machine Learning of Multireference Character across Known Transition Metal Complex Ligands. Journal of Chemical Theory and Computation, 2022, 18, 4836-4845.	2.3	4
115	Quantifying the Longâ€Range Coupling of Electronic Properties in Proteins with ab initio Molecular Dynamics**. Chemistry Methods, 2021, 1, 362-373.	1.8	3
116	Computational Scaling Relationships Predict Experimental Activity and Rate-Limiting Behavior in Homogeneous Water Oxidation. Inorganic Chemistry, 2022, 61, 2186-2197.	1.9	3
117	Quantum-Mechanical/Molecular-Mechanical (QM/MM) Simulations for Understanding Enzyme Dynamics. Methods in Molecular Biology, 2022, 2397, 227-248.	0.4	2
118	Molecular orbital projectors in non-empirical jmDFT recover exact conditions in transition-metal chemistry. Journal of Chemical Physics, 2022, 156, 184112.	1.2	2
119	Ligand Additivity and Divergent Trends in Two Types of Delocalization Errors from Approximate Density Functional Theory. Journal of Physical Chemistry Letters, 2022, 13, 4549-4555.	2.1	2
120	Mechanistic Studies of a Skatole-Forming Glycyl Radical Enzyme Suggest Reaction Initiation via Hydrogen Atom Transfer. Journal of the American Chemical Society, 2022, 144, 11110-11119.	6.6	2
121	Reply to â€œComment on â€˜Evaluating Unexpectedly Short Non-covalent Distances in X-ray Crystal Structures of Proteins with Electronic Structure Analysisâ€™â€•. Journal of Chemical Information and Modeling, 2019, 59, 3609-3610.	2.5	1
122	Protein Dynamics and Substrate Protonation States Mediate the Catalytic Action of trans-4-Hydroxy-l-Proline Dehydratase. Journal of Physical Chemistry B, 2021, 125, 7774-7784.	1.2	1
123	Redox Electrodes: Anion-Selective Redox Electrodes: Electrochemically Mediated Separation with Heterogeneous Organometallic Interfaces (Adv. Funct. Mater. 20/2016). Advanced Functional Materials, 2016, 26, 3552-3552.	7.8	0
124	Electronic Structure Origins of Surface-Dependent Growth in IIIâ€“V Quantum Dots. , 0, , .		0
125	Electronic Structure Origins of Surface-Dependent Growth in IIIâ€“V Quantum Dots. , 0, , .		0