Heather J Kulik

List of Publications by Year
in descending order

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Version: 2024-02-01

125 papers	6,168 citations	70961 41 h-index	79541 73 g-index
168 all docs	168 docs citations	168 times ranked	6004 citing authors

#	Article	IF	Citations
1	What's Left for a Computational Chemist To Do in the Age of Machine Learning?. Israel Journal of Chemistry, 2022, 62, .	1.0	6
2	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
3	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
4	Quantum-Mechanical/Molecular-Mechanical (QM/MM) Simulations for Understanding Enzyme Dynamics. Methods in Molecular Biology, 2022, 2397, 227-248.	0.4	2
5	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
6	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
7	Machine learning reveals key ion selectivity mechanisms in polymeric membranes with subnanometer pores. Science Advances, 2022, 8, eabl5771.	4.7	45
8	Representations and strategies for transferable machine learning improve model performance in chemical discovery. Journal of Chemical Physics, 2022, 156, 074101.	1.2	11
9	Computational Scaling Relationships Predict Experimental Activity and Rate-Limiting Behavior in Homogeneous Water Oxidation. Inorganic Chemistry, 2022, 61, 2186-2197.	1.9	3
10	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
11	Irreversible synthesis of an ultrastrong two-dimensional polymeric material. Nature, 2022, 602, 91-95.	13.7	42
12	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
13	Machine Learning for the Discovery, Design, and Engineering of Materials. Annual Review of Chemical and Biomolecular Engineering, 2022, 13, 405-429.	3.3	10
14	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
15	MOFSimplify, machine learning models with extracted stability data of three thousand metalâ€“organic frameworks. Scientific Data, 2022, 9, 74.	2.4	34
16	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
17	Are Vanadium Intermediates Suitable Mimics in Non-Heme Iron Enzymes? An Electronic Structure Analysis. ACS Catalysis, 2022, 12, 5489-5501.	5.5	5
18	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

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19	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
20	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
21	Molecular orbital projectors in non-empirical jmDFT recover exact conditions in transition-metal chemistry. Journal of Chemical Physics, 2022, 156, 184112.	1.2	2
22	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
23	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
24	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
25	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
26	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
27	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
28	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
29	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
30	Biochemical and crystallographic investigations into isonitrile formation by a nonheme iron-dependent oxidase/decarboxylase. Journal of Biological Chemistry, 2021, 296, 100231.	1.6	16
31	Molecular DFT+U: A Transferable, Low-Cost Approach to Eliminate Delocalization Error. Journal of Physical Chemistry Letters, 2021, 12, 3633-3640.	2.1	9
32	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
33	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
34	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
35	Computational Discovery of Transition-metal Complexes: From High-throughput Screening to Machine Learning. Chemical Reviews, 2021, 121, 9927-10000.	23.0	110
36	Quantifying the Longâ€Range Coupling of Electronic Properties in Proteins with ab initio Molecular Dynamics**. Chemistry Methods, 2021, 1, 362-373.	1.8	3

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37	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
38	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
39	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
40	Deciphering Cryptic Behavior in Bimetallic Transition-Metal Complexes with Machine Learning. Journal of Physical Chemistry Letters, 2021, 12, 9812-9820.	2.1	4
41	Navigating Transition-Metal Chemical Space: Artificial Intelligence for First-Principles Design. Accounts of Chemical Research, 2021, 54, 532-545.	7.6	34
42	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
43	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
44	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
45	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
46	Enumeration of de novo inorganic complexes for chemical discovery and machine learning. Molecular Systems Design and Engineering, 2020, 5, 139-152.	1.7	23
47	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
48	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
49	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
50	Understanding the diversity of the metal-organic framework ecosystem. Nature Communications, 2020, 11, 4068.	5.8	282
51	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
52	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
53	Why Conventional Design Rules for Câ€“H Activation Fail for Open-Shell Transition-Metal Catalysts. ACS Catalysis, 2020, 10, 15033-15047.	5.5	30
54	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

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55	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
56	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
57	Seeing Is Believing: Experimental Spin States from Machine Learning Model Structure Predictions. Journal of Physical Chemistry A, 2020, 124, 3286-3299.	1.1	48
58	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
59	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
60	A quantitative uncertainty metric controls error in neural network-driven chemical discovery. Chemical Science, 2019, 10, 7913-7922.	3.7	129
61	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
62	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
63	Revealing quantum mechanical effects in enzyme catalysis with large-scale electronic structure simulation. Reaction Chemistry and Engineering, 2019, 4, 298-315.	1.9	33
64	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
65	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
66	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
67	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
68	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
69	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
70	Bridging the Homogeneous-Heterogeneous Divide: Modeling Spin for Reactivity in Single Atom Catalysis. Frontiers in Chemistry, 2019, 7, 219.	1.8	34
71	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
72	Protection of tissue physicochemical properties using polyfunctional crosslinkers. Nature Biotechnology, 2019, 37, 73-83.	9.4	262

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73	Coding solvation: challenges and opportunities. International Journal of Quantum Chemistry, 2019, 119, e25839.	1.0	4
74	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
75	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
76	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
77	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
78	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
79	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
80	Strategies and Software for Machine Learning Accelerated Discovery in Transition Metal Chemistry. Industrial & Engineering Chemistry Research, 2018, 57, 13973-13986.	1.8	104
81	Electronic Structure Origins of Surface-Dependent Growth in IIIâ€“V Quantum Dots. Chemistry of Materials, 2018, 30, 7154-7165.	3.2	25
82	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
83	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
84	Systematic Quantum Mechanical Region Determination in QM/MM Simulation. Journal of Chemical Theory and Computation, 2017, 13, 563-576.	2.3	72
85	Predicting electronic structure properties of transition metal complexes with neural networks. Chemical Science, 2017, 8, 5137-5152.	3.7	152
86	Leveraging Cheminformatics Strategies for Inorganic Discovery: Application to Redox Potential Design. Industrial & Engineering Chemistry Research, 2017, 56, 4898-4910.	1.8	45
87	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
88	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
89	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
90	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

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91	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
92	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
93	Computational Investigation of the Interplay of Substrate Positioning and Reactivity in Catechol O-Methyltransferase. PLoS ONE, 2016, 11, e0161868.	1.1	36
94	Anionâ€Selective Redox Electrodes: Electrochemically Mediated Separation with Heterogeneous Organometallic Interfaces. Advanced Functional Materials, 2016, 26, 3394-3404.	7.8	106
95	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
96	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
97	Global and local curvature in density functional theory. Journal of Chemical Physics, 2016, 145, 054109.	1.2	38
98	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
99	Computational Discovery of Hydrogen Bond Design Rules for Electrochemical Ion Separation. Chemistry of Materials, 2016, 28, 6207-6218.	3.2	17
100	molSimplify: A toolkit for automating discovery in inorganic chemistry. Journal of Computational Chemistry, 2016, 37, 2106-2117.	1.5	127
101	Predicting the Stability of Fullerene Allotropes Throughout the Periodic Table. Journal of Physical Chemistry C, 2016, 120, 17035-17045.	1.5	7
102	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
103	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
104	Perspective: Treating electron over-delocalization with the DFT+U method. Journal of Chemical Physics, 2015, 142, 240901.	1.2	154
105	Ab Initio Screening Approach for the Discovery of Lignin Polymer Breaking Pathways. Journal of Physical Chemistry A, 2015, 119, 6551-6562.	1.1	16
106	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
107	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
108	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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109	Towards quantifying the role of exact exchange in predictions of transition metal complex properties. Journal of Chemical Physics, 2015, 143, 034104.	1.2	93
110	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
111	Mechanically triggered heterolytic unzipping of a low-ceiling-temperature polymer. Nature Chemistry, 2014, 6, 623-628.	6.6	198
112	Substrate Placement Influences Reactivity in Non-heme Fe(II) Halogenases and Hydroxylases. Journal of Biological Chemistry, 2013, 288, 11233-11241.	1.6	51
113	Ab Initio Quantum Chemistry for Protein Structures. Journal of Physical Chemistry B, 2012, 116, 12501-12509.	1.2	99
114	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
115	Transition-metal dioxides: A case for the intersite term in Hubbard-model functionals. Journal of Chemical Physics, 2011, 134, 094103.	1.2	55
116	Accurate potential energy surfaces with a DFT+$U(mathbf {R})$U(R) approach. Journal of Chemical Physics, 2011, 135, 194105.	1.2	63
117	Designing small-molecule catalysts for CO2 capture. Energy Procedia, 2011, 4, 817-823.	1.8	18
118	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
119	Local Effects in the X-ray Absorption Spectrum of Salt Water. Journal of Physical Chemistry B, 2010, 114, 9594-9601.	1.2	41
120	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
121	First-Principles Study of Non-heme Fe(II) Halogenase SyrB2 Reactivity. Journal of the American Chemical Society, 2009, 131, 14426-14433.	6.6	50
122	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
123	Density Functional Theory in Transition-Metal Chemistry: A Self-Consistent HubbardUApproach. Physical Review Letters, 2006, 97, 103001.	2.9	526
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