Heather J Kulik

List of Publications by Year in Descending Order

113 papers	3,832 citations	35 h-index	59 g-index
168 ext. papers	5,037 ext. citations	8.2 avg, IF	6.49 L-index

#	Paper	IF	Citations
113	Machine learning reveals key ion selectivity mechanisms in polymeric membranes with subnanometer pores.. *Science Advances*, **2022**, 8, eabl5771	14.3	6
112	Representations and strategies for transferable machine learning improve model performance in chemical discovery.. *Journal of Chemical Physics*, **2022**, 156, 074101	3.9	1
111	Computational Scaling Relationships Predict Experimental Activity and Rate-Limiting Behavior in Homogeneous Water Oxidation.. *Inorganic Chemistry*, **2022**,	5.1	1
110	Eliminating Delocalization Error to Improve Heterogeneous Catalysis Predictions with Molecular DFT + .. *Journal of Chemical Theory and Computation*, **2022**,	6.4	2
109	Irreversible synthesis of an ultrastrong two-dimensional polymeric material.. *Nature*, **2022**, 602, 91-95	50.4	3
108	Quantum-Mechanical/Molecular-Mechanical (QM/MM) Simulations for Understanding Enzyme Dynamics. *Methods in Molecular Biology*, **2022**, 2397, 227-248	1.4	
107	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	5.4	1
106	MOFSimplify, machine learning models with extracted stability data of three thousand metal-organic frameworks.. *Scientific Data*, **2022**, 9, 74	8.2	1
105	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	13.1	0
104	Are Vanadium Intermediates Suitable Mimics in Non-Heme Iron Enzymes? An Electronic Structure Analysis. *ACS Catalysis*, **2022**, 12, 5489-5501	13.1	0
103	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	3.9	1
102	Molecular orbital projectors in non-empirical jmDFT recover exact conditions in transition-metal chemistry.. *Journal of Chemical Physics*, **2022**, 156, 184112	3.9	
101	Ligand Additivity and Divergent Trends in Two Types of Delocalization Errors from Approximate Density Functional Theory.. *Journal of Physical Chemistry Letters*, **2022**, 4549-4555	6.4	1
100	Quantum Chemistry Common Driver and Databases (QCDB) and Quantum Chemistry Engine (QCEngine): Automation and interoperability among computational chemistry programs. *Journal of Chemical Physics*, **2021**, 155, 204801	3.9	3
99	Using Machine Learning and Data Mining to Leverage Community Knowledge for the Engineering of Stable Metal-Organic Frameworks. *Journal of the American Chemical Society*, **2021**, 143, 17535-17547	16.4	13
98	Molecular DFT+U: A Transferable, Low-Cost Approach to Eliminate Delocalization Error. *Journal of Physical Chemistry Letters*, **2021**, 12, 3633-3640	6.4	4
97	Putting Density Functional Theory to the Test in Machine-Learning-Accelerated Materials Discovery. *Journal of Physical Chemistry Letters*, **2021**, 12, 4628-4637	6.4	16

96	Protein Dynamics and Substrate Protonation States Mediate the Catalytic Action of -4-Hydroxy-l-Proline Dehydratase. *Journal of Physical Chemistry B*, **2021**, 125, 7774-7784	3.4	
95	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	8.4	7
94	Biochemical and crystallographic investigations into isonitrile formation by a nonheme iron-dependent oxidase/decarboxylase. *Journal of Biological Chemistry*, **2021**, 296, 100231	5.4	4
93	Computational Discovery of Transition-metal Complexes: From High-throughput Screening to Machine Learning. *Chemical Reviews*, **2021**, 121, 9927-10000	68.1	26
92	Quantifying the Long-Range Coupling of Electronic Properties in Proteins with ab initio Molecular Dynamics**. *Chemistry Methods*, **2021**, 1, 362-373		0
91	Spectroscopically Guided Simulations Reveal Distinct Strategies for Positioning Substrates to Achieve Selectivity in Nonheme Fe(II)/□Ketoglutarate-Dependent Halogenases. *ACS Catalysis*, **2021**, 11, 12394-12408	13.1	4
90	Mapping the Origins of Surface- and Chemistry-Dependent Doping Trends in III□V Quantum Dots with Density Functional Theory. *Chemistry of Materials*, **2021**, 33, 7113-7123	9.6	1
89	Molecular basis of C-S bond cleavage in the glycyl radical enzyme isethionate sulfite-lyase. *Cell Chemical Biology*, **2021**, 28, 1333-1346.e7	8.2	5
88	Deciphering Cryptic Behavior in Bimetallic Transition-Metal Complexes with Machine Learning. *Journal of Physical Chemistry Letters*, **2021**, 12, 9812-9820	6.4	2
87	Harder, better, faster, stronger: Large-scale QM and QM/MM for predictive modeling in enzymes and proteins. *Current Opinion in Structural Biology*, **2021**, 72, 9-17	8.1	7
86	Navigating Transition-Metal Chemical Space: Artificial Intelligence for First-Principles Design. *Accounts of Chemical Research*, **2021**, 54, 532-545	24.3	14
85	Machine learning to tame divergent density functional approximations: a new path to consensus materials design principles. *Chemical Science*, **2021**, 12, 13021-13036	9.4	9
84	Why Conventional Design Rules for C□H Activation Fail for Open-Shell Transition-Metal Catalysts. *ACS Catalysis*, **2020**, 10, 15033-15047	13.1	12
83	Data-Driven Approaches Can Overcome the Cost-Accuracy Trade-Off in Multireference Diagnostics. *Journal of Chemical Theory and Computation*, **2020**, 16, 4373-4387	6.4	15
82	Uncovering Alternate Pathways to Nafion Membrane Degradation in Fuel Cells with First-Principles Modeling. *Journal of Physical Chemistry C*, **2020**, 124, 15094-15106	3.8	3
81	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	16.8	58
80	Seeing Is Believing: Experimental Spin States from Machine Learning Model Structure Predictions. *Journal of Physical Chemistry A*, **2020**, 124, 3286-3299	2.8	28
79	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	6.4	13

78	Machine Learning in Chemistry **2020**,		14
77	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	6.4	11
76	Ionization behavior of nanoporous polyamide membranes. *Proceedings of the National Academy of Sciences of the United States of America*, **2020**, 117, 30191-30200	11.5	21
75	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	3.6	13
74	Understanding the diversity of the metal-organic framework ecosystem. *Nature Communications*, **2020**, 11, 4068	17.4	92
73	Rapid Detection of Strong Correlation with Machine Learning for Transition-Metal Complex High-Throughput Screening. *Journal of Physical Chemistry Letters*, **2020**, 11, 8067-8076	6.4	17
72	Semi-supervised Machine Learning Enables the Robust Detection of Multireference Character at Low Cost. *Journal of Physical Chemistry Letters*, **2020**, 11, 6640-6648	6.4	22
71	Making machine learning a useful tool in the accelerated discovery of transition metal complexes. *Wiley Interdisciplinary Reviews: Computational Molecular Science*, **2020**, 10, e1439	7.9	25
70	Enumeration of de novo inorganic complexes for chemical discovery and machine learning. *Molecular Systems Design and Engineering*, **2020**, 5, 139-152	4.6	15
69	Reply to "Comment on '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, 3609-3610	6.1	1
68	Revealing quantum mechanical effects in enzyme catalysis with large-scale electronic structure simulation. *Reaction Chemistry and Engineering*, **2019**, 4, 298-315	4.9	21
67	Quantum Mechanical Description of Electrostatics Provides a Unified Picture of Catalytic Action Across Methyltransferases. *Journal of Physical Chemistry Letters*, **2019**, 10, 3779-3787	6.4	11
66	Critical Knowledge Gaps in Mass Transport through Single-Digit Nanopores: A Review and Perspective. *Journal of Physical Chemistry C*, **2019**, 123, 21309-21326	3.8	121
65	Non-empirical, low-cost recovery of exact conditions with model-Hamiltonian inspired expressions in jmDFT. *Journal of Chemical Physics*, **2019**, 150, 154115	3.9	9
64	The Protein's Role in Substrate Positioning and Reactivity for Biosynthetic Enzyme Complexes: The Case of SyrB2/SyrB1. *ACS Catalysis*, **2019**, 9, 4930-4943	13.1	15
63	Learning from Failure: Predicting Electronic Structure Calculation Outcomes with Machine Learning Models. *Journal of Chemical Theory and Computation*, **2019**, 15, 2331-2345	6.4	45
62	Designing in the Face of Uncertainty: Exploiting Electronic Structure and Machine Learning Models for Discovery in Inorganic Chemistry. *Inorganic Chemistry*, **2019**, 58, 10592-10606	5.1	56
61	Bridging the Homogeneous-Heterogeneous Divide: Modeling Spin for Reactivity in Single Atom Catalysis. *Frontiers in Chemistry*, **2019**, 7, 219	5	19

60	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	6.1	21
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	6.4	19
58	A quantitative uncertainty metric controls error in neural network-driven chemical discovery. *Chemical Science*, **2019**, 10, 7913-7922	9.4	83
57	Machine Learning Accelerates the Discovery of Design Rules and Exceptions in Stable Metal□Oxo Intermediate Formation. *ACS Catalysis*, **2019**, 9, 8243-8255	13.1	47
56	Anthracene as a Launchpad for a Phosphinidene Sulfide and for Generation of a Phosphorus-Sulfur Material Having the Composition PS, a Vulcanized Red Phosphorus That Is Yellow. *Journal of the American Chemical Society*, **2019**, 141, 431-440	16.4	17
55	Exploiting graphical processing units to enable quantum chemistry calculation of large solvated molecules with conductor-like polarizable continuum models. *International Journal of Quantum Chemistry*, **2019**, 119, e25760	2.1	23
54	When Is Ligand p K a Good Descriptor for Catalyst Energetics? In Search of Optimal CO Hydration Catalysts. *Journal of Physical Chemistry A*, **2018**, 122, 4579-4590	2.8	11
53	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	6.4	110
52	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	6.4	37
51	Large-scale QM/MM free energy simulations of enzyme catalysis reveal the influence of charge transfer. *Physical Chemistry Chemical Physics*, **2018**, 20, 20650-20660	3.6	23
50	Protection of tissue physicochemical properties using polyfunctional crosslinkers. *Nature Biotechnology*, **2018**,	44.5	123
49	Understanding and Breaking Scaling Relations in Single-Site Catalysis: Methane to Methanol Conversion by FeIV?O. *ACS Catalysis*, **2018**, 8, 975-986	13.1	84
48	MODELING MECHANOCHEMISTRY FROM FIRST PRINCIPLES. *Reviews in Computational Chemistry*, **2018**, 265-311		0
47	Strategies and Software for Machine Learning Accelerated Discovery in Transition Metal Chemistry. *Industrial & Engineering Chemistry Research*, **2018**, 57, 13973-13986	3.9	70
46	Electronic Structure Origins of Surface-Dependent Growth in III□V Quantum Dots. *Chemistry of Materials*, **2018**, 30, 7154-7165	9.6	16
45	Ligand-Field-Dependent Behavior of Meta-GGA Exchange in Transition-Metal Complex Spin-State Ordering. *Journal of Physical Chemistry A*, **2017**, 121, 874-884	2.8	46
44	Systematic Quantum Mechanical Region Determination in QM/MM Simulation. *Journal of Chemical Theory and Computation*, **2017**, 13, 563-576	6.4	55
43	Predicting electronic structure properties of transition metal complexes with neural networks. *Chemical Science*, **2017**, 8, 5137-5152	9.4	112

42	Leveraging Cheminformatics Strategies for Inorganic Discovery: Application to Redox Potential Design. *Industrial & Engineering Chemistry Research*, **2017**, 56, 4898-4910	3.9	36
41	Harnessing Organic Ligand Libraries for First-Principles Inorganic Discovery: Indium Phosphide Quantum Dot Precursor Design Strategies. *Chemistry of Materials*, **2017**, 29, 3632-3643	9.6	21
40	Depolymerization Pathways for Branching Lignin Spirodienone Units Revealed with ab Initio Steered Molecular Dynamics. *Journal of Physical Chemistry A*, **2017**, 121, 532-543	2.8	10
39	Density functional theory for modelling large molecular adsorbate surface interactions: a mini-review and worked example. *Molecular Simulation*, **2017**, 43, 327-345	2	34
38	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	6.4	34
37	Resolving Transition Metal Chemical Space: Feature Selection for Machine Learning and Structure-Property Relationships. *Journal of Physical Chemistry A*, **2017**, 121, 8939-8954	2.8	107
36	Communication: Recovering the flat-plane condition in electronic structure theory at semi-local DFT cost. *Journal of Chemical Physics*, **2017**, 147, 191101	3.9	21
35	Computational Discovery of Hydrogen Bond Design Rules for Electrochemical Ion Separation. *Chemistry of Materials*, **2016**, 28, 6207-6218	9.6	16
34	molSimplify: A toolkit for automating discovery in inorganic chemistry. *Journal of Computational Chemistry*, **2016**, 37, 2106-17	3.5	76
33	Predicting the Stability of Fullerene Allotropes Throughout the Periodic Table. *Journal of Physical Chemistry C*, **2016**, 120, 17035-17045	3.8	7
32	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	6.4	50
31	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	3.8	18
30	Computational Investigation of the Interplay of Substrate Positioning and Reactivity in Catechol O-Methyltransferase. *PLoS ONE*, **2016**, 11, e0161868	3.7	23
29	Anion-Selective Redox Electrodes: Electrochemically Mediated Separation with Heterogeneous Organometallic Interfaces. *Advanced Functional Materials*, **2016**, 26, 3394-3404	15.6	71
28	Adapting DFT+U for the Chemically Motivated Correction of Minimal Basis Set Incompleteness. *Journal of Physical Chemistry A*, **2016**, 120, 5939-49	2.8	16
27	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	15.6	
26	Global and local curvature in density functional theory. *Journal of Chemical Physics*, **2016**, 145, 054109	3.9	34
25	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	3.4	110

24	Quantum Chemistry for Solvated Molecules on Graphical Processing Units Using Polarizable Continuum Models. *Journal of Chemical Theory and Computation*, **2015**, 11, 3131-44	6.4	69
23	Mediation of donor-acceptor distance in an enzymatic methyl transfer reaction. *Proceedings of the National Academy of Sciences of the United States of America*, **2015**, 112, 7954-9	11.5	55
22	Discovering Amorphous Indium Phosphide Nanostructures with High-Temperature ab Initio Molecular Dynamics. *Journal of Physical Chemistry C*, **2015**, 119, 23238-23249	3.8	11
21	Towards quantifying the role of exact exchange in predictions of transition metal complex properties. *Journal of Chemical Physics*, **2015**, 143, 034104	3.9	77
20	Perspective: Treating electron over-delocalization with the DFT+U method. *Journal of Chemical Physics*, **2015**, 142, 240901	3.9	113
19	Ab Initio Screening Approach for the Discovery of Lignin Polymer Breaking Pathways. *Journal of Physical Chemistry A*, **2015**, 119, 6551-62	2.8	12
18	Mechanically triggered heterolytic unzipping of a low-ceiling-temperature polymer. *Nature Chemistry*, **2014**, 6, 623-8	17.6	157
17	Developing an approach for first-principles catalyst design: application to carbon-capture catalysis. *Acta Crystallographica Section C, Structural Chemistry*, **2014**, 70, 123-31	0.8	12
16	Substrate placement influences reactivity in non-heme Fe(II) halogenases and hydroxylases. *Journal of Biological Chemistry*, **2013**, 288, 11233-41	5.4	37
15	Ab initio quantum chemistry for protein structures. *Journal of Physical Chemistry B*, **2012**, 116, 12501-9	3.4	88
14	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, 2653-8	6.4	34
13	Accurate potential energy surfaces with a DFT+U(R) approach. *Journal of Chemical Physics*, **2011**, 135, 194105	3.9	56
12	Transition-metal dioxides: a case for the intersite term in Hubbard-model functionals. *Journal of Chemical Physics*, **2011**, 134, 094103	3.9	43
11	Designing small-molecule catalysts for CO2 capture. *Energy Procedia*, **2011**, 4, 817-823	2.3	14
10	Systematic study of first-row transition-metal diatomic molecules: a self-consistent DFT+U approach. *Journal of Chemical Physics*, **2010**, 133, 114103	3.9	73
9	Local effects in the X-ray absorption spectrum of salt water. *Journal of Physical Chemistry B*, **2010**, 114, 9594-601	3.4	38
8	Electronic Structure and Reactivity of Transition Metal Complexes **2010**, 433-455		3
7	Ab initio investigation of high multiplicity ⊞⊞ optical transitions in the spectra of CN and isoelectronic species. *Journal of Molecular Spectroscopy*, **2009**, 258, 6-12	1.3	8

6	First-principles study of non-heme Fe(II) halogenase SyrB2 reactivity. *Journal of the American Chemical Society*, **2009**, 131, 14426-33	16.4	43
5	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	3.9	61
4	Density functional theory in transition-metal chemistry: a self-consistent Hubbard U approach. *Physical Review Letters*, **2006**, 97, 103001	7.4	421
3	What's Left for a Computational Chemist To Do in the Age of Machine Learning?. *Israel Journal of Chemistry*,	3.4	1
2	The Effect of Hartree-Fock Exchange on Scaling Relations and Reaction Energetics for C□H Activation Catalysts. *Topics in Catalysis*,1	2.3	3
1	Influence of the Greater Protein Environment on the Electrostatic Potential in Metalloenzyme Active Sites: the Case of Formate Dehydrogenase		2