

# Johannes Hachmann

## List of Publications by Year in descending order

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Version: 2024-02-01

29  
papers

2,375  
citations

394421

19  
h-index

526287

27  
g-index

33  
all docs

33  
docs citations

33  
times ranked

2712  
citing authors

#	ARTICLE	IF	CITATIONS
1	Metrics for Benchmarking and Uncertainty Quantification: Quality, Applicability, and Best Practices for Machine Learning in Chemistry. Trends in Chemistry, 2021, 3, 146-156.	8.5	37
2	Open Chemistry, <sc>JupyterLab</sc>, <sc>REST</sc>, and quantum chemistry. International Journal of Quantum Chemistry, 2021, 121, .	2.0	7
3	<i>The Journal of Physical Chemistry A</i>/<i>B</i>/<i>C</i> Virtual Special Issue on Machine Learning in Physical Chemistry. Journal of Physical Chemistry B, 2020, 124, 9767-9772.	2.6	2
4	<i>The Journal of Physical Chemistry A</i>/<i>B</i>/<i>C</i> Virtual Special Issue on Machine Learning in Physical Chemistry. Journal of Physical Chemistry A, 2020, 124, 9113-9118.	2.5	2
5	<i>The Journal of Physical Chemistry A</i>/<i>B</i>/<i>C</i> Virtual Special Issue on Machine Learning in Physical Chemistry. Journal of Physical Chemistry C, 2020, 124, 24033-24038.	3.1	1
6	<i>ChemML</i>: A machine learning and informatics program package for the analysis, mining, and modeling of chemical and materials data. Wiley Interdisciplinary Reviews: Computational Molecular Science, 2020, 10, e1458.	14.6	41
7	High-Throughput Computational Studies in Catalysis and Materials Research, and Their Impact on Rational Design. , 2020, , 1-44.		1
8	A deep neural network model for packing density predictions and its application in the study of 1.5 million organic molecules. Chemical Science, 2019, 10, 8374-8383.	7.4	30
9	Benchmarking DFT approaches for the calculation of polarizability inputs for refractive index predictions in organic polymers. Physical Chemistry Chemical Physics, 2019, 21, 4452-4460.	2.8	24
10	Accelerated Discovery of High-Refractive-Index Polyimides via <i>First-Principles</i> Molecular Modeling, Virtual High-Throughput Screening, and Data Mining. Journal of Physical Chemistry C, 2019, 123, 14610-14618.	3.1	36
11	Advances of machine learning in molecular modeling and simulation. Current Opinion in Chemical Engineering, 2019, 23, 51-57.	7.8	84
12	Machine learning and data science in materials design: a themed collection. Molecular Systems Design and Engineering, 2018, 3, 429-430.	3.4	6
13	Combining first-principles and data modeling for the accurate prediction of the refractive index of organic polymers. Journal of Chemical Physics, 2018, 148, 241712.	3.0	33
14	Roaming-like Mechanism for Dehydration of Diol Radicals. Journal of Physical Chemistry A, 2018, 122, 9738-9754.	2.5	7
15	Building and deploying a cyberinfrastructure for the data-driven design of chemical systems and the exploration of chemical space. Molecular Simulation, 2018, 44, 921-929.	2.0	28
16	Revisiting the polytopal rearrangements in penta-coordinate d<sup>7</sup>-metallocomplexes: modified Berry pseudorotation, octahedral switch, and butterfly isomerization. Chemical Science, 2017, 8, 5512-5525.	7.4	18
17	The Harvard organic photovoltaic dataset. Scientific Data, 2016, 3, 160086.	5.3	85
18	Lead candidates for high-performance organic photovoltaics from high-throughput quantum chemistry – the Harvard Clean Energy Project. Energy and Environmental Science, 2014, 7, 698-704.	30.8	189

#	ARTICLE	IF	CITATIONS
19	Organic Photovoltaics. , 2013, , 423-442.		10
20	Accelerated computational discovery of high-performance materials for organic photovoltaics by means of cheminformatics. Energy and Environmental Science, 2011, 4, 4849.	30.8	169
21	The Harvard Clean Energy Project: Large-Scale Computational Screening and Design of Organic Photovoltaics on the World Community Grid. Journal of Physical Chemistry Letters, 2011, 2, 2241-2251.	4.6	470
22	A Theoretical Study of the $3d^2$ Complexes: Structure, Magnetism, and Oxidation States. ChemPhysChem, 2011, 12, 3236-3244.	2.1	7
23	Analytic response theory for the density matrix renormalization group. Journal of Chemical Physics, 2009, 130, 184111.	3.0	55
24	Orbital optimization in the density matrix renormalization group, with applications to polyenes and $\beta$ -carotene. Journal of Chemical Physics, 2008, 128, 144117.	3.0	288
25	An Introduction to the Density Matrix Renormalization Group Ansatz in Quantum Chemistry. Progress in Theoretical Chemistry and Physics, 2008, , 49-65.	0.2	57
26	The radical character of the acenes: A density matrix renormalization group study. Journal of Chemical Physics, 2007, 127, 134309.	3.0	421
27	Targeted excited state algorithms. Journal of Chemical Physics, 2007, 127, 084109.	3.0	63
28	Multireference correlation in long molecules with the quadratic scaling density matrix renormalization group. Journal of Chemical Physics, 2006, 125, 144101.	3.0	174
29	The nodes of Hartree-Fock wavefunctions and their orbitals. Chemical Physics Letters, 2004, 392, 55-61.	2.6	24