# Johannes Hachmann

List of Publications by Year
in descending order

| 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 | 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 |
| 2 | The radical character of the acenes: A density matrix renormalization group study. Journal of Chemical Physics, 2007, 127, 134309. | 3.0 | 421 |
| 3 | 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 |
| 4 | Lead candidates for high-performance organic photovoltaics from high-throughput quantum chemistry â€" the Harvard Clean Energy Project. Energy and Environmental Science, 2014, 7, 698-704. | 30.8 | 189 |
| 5 | Multireference correlation in long molecules with the quadratic scaling density matrix renormalization group. Journal of Chemical Physics, 2006, 125, 144101. | 3.0 | 174 |
| 6 | Accelerated computational discovery of high-performance materials for organic photovoltaics by means of cheminformatics. Energy and Environmental Science, 2011, 4, 4849. | 30.8 | 169 |
| 7 | The Harvard organic photovoltaic dataset. Scientific Data, 2016, 3, 160086. | 5.3 | 85 |
| 8 | Advances of machine learning in molecular modeling and simulation. Current Opinion in Chemical Engineering, 2019, 23, 51-57. | 7.8 | 84 |
| 9 | Targeted excited state algorithms. Journal of Chemical Physics, 2007, 127, 084109. | 3.0 | 63 |
| 10 | An Introduction to the Density Matrix Renormalization Group Ansatz in Quantum Chemistry. Progress in Theoretical Chemistry and Physics, 2008, , 49-65. | 0.2 | 57 |
| 11 | Analytic response theory for the density matrix renormalization group. Journal of Chemical Physics, 2009, 130, 184111. | 3.0 | 55 |
| 12 | <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 |
| 13 | 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 |
| 14 | 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 |
| 15 | 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 |
| 16 | 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 |
| 17 | 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 |
| 18 | The nodes of Hartreeâ€"Fock wavefunctions and their orbitals. Chemical Physics Letters, 2004, 392, 55-61. | 2.6 | 24 |

| # | ARTICLE | IF | CITATIONS |
|---|---------|-----|-----------|
| 19 | 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 |
| 20 | Revisiting the polytopal rearrangements in penta-coordinate $d^7$-metallocomplexes: modified Berry pseudorotation, octahedral switch, and butterfly isomerization. Chemical Science, 2017, 8, 5512-5525. | 7.4 | 18 |
| 21 | Organic Photovoltaics. , 2013, , 423-442. | | 10 |
| 22 | A Theoretical Study of the 3dâ€M(smif)$_2$Complexes: Structure, Magnetism, and Oxidation States. ChemPhysChem, 2011, 12, 3236-3244. | 2.1 | 7 |
| 23 | Roaming-like Mechanism for Dehydration of Diol Radicals. Journal of Physical Chemistry A, 2018, 122, 9738-9754. | 2.5 | 7 |
| 24 | Open Chemistry, <scp>JupyterLab</scp>, <scp>REST</scp>, and quantum chemistry. International Journal of Quantum Chemistry, 2021, 121, . | 2.0 | 7 |
| 25 | Machine learning and data science in materials design: a themed collection. Molecular Systems Design and Engineering, 2018, 3, 429-430. | 3.4 | 6 |
| 26 | <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 |
| 27 | <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 |
| 28 | <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 |
| 29 | High-Throughput Computational Studies in Catalysis and Materials Research, and Their Impact on Rational Design. , 2020, , 1-44. | | 1 |