Daniel G A Smith

List of Publications by Year
in descending order

27	2,633	394421	526287
papers	citations	19 h-index	27 g-index

34	34	34	3310
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	<scp>Psi4</scp> 1.1: An Open-Source Electronic Structure Program Emphasizing Automation, Advanced Libraries, and Interoperability. Journal of Chemical Theory and Computation, 2017, 13, 3185-3197.	5.3	961
2	P<scp>SI4</scp> 1.4: Open-source software for high-throughput quantum chemistry. Journal of Chemical Physics, 2020, 152, 184108.	3.0	440
3	Revised Damping Parameters for the D3 Dispersion Correction to Density Functional Theory. Journal of Physical Chemistry Letters, 2016, 7, 2197-2203.	4.6	305
4	P<scp>si</scp>4N<scp>um</scp>P<scp>y</scp>: An Interactive Quantum Chemistry Programming Environment for Reference Implementations and Rapid Development. Journal of Chemical Theory and Computation, 2018, 14, 3504-3511.	5.3	106
5	The BioFragment Database (BFDb): An open-data platform for computational chemistry analysis of noncovalent interactions. Journal of Chemical Physics, 2017, 147, 161727.	3.0	82
6	Development and Benchmarking of Open Force Field v1.0.0â€"the Parsley Small-Molecule Force Field. Journal of Chemical Theory and Computation, 2021, 17, 6262-6280.	5.3	80
7	Perspective: Computational chemistry software and its advancement as illustrated through three grand challenge cases for molecular science. Journal of Chemical Physics, 2018, 149, 180901.	3.0	72
8	PES-Learn: An Open-Source Software Package for the Automated Generation of Machine Learning Models of Molecular Potential Energy Surfaces. Journal of Chemical Theory and Computation, 2019, 15, 4386-4398.	5.3	51
9	Benchmarking the CO₂ Adsorption Energy on Carbon Nanotubes. Journal of Physical Chemistry C, 2015, 119, 4934-4948.	3.1	47
10	Highly accurate potential energy surface for the Heâ€“H2 dimer. Journal of Chemical Physics, 2013, 139, 144305.	3.0	46
11	opt_einsum - A Python package for optimizing contraction order for einsum-like expressions. Journal of Open Source Software, 2018, 3, 753.	4.6	46
12	Basis Set Convergence of the Post-CCSD(T) Contribution to Noncovalent Interaction Energies. Journal of Chemical Theory and Computation, 2014, 10, 3140-3150.	5.3	43
13	The <scp>MolSSI</scp> QCA<scp>rchive</scp> project: An openâ€source platform to compute, organize, and share quantum chemistry data. Wiley Interdisciplinary Reviews: Computational Molecular Science, 2021, 11, e1491.	14.6	42
14	OrbNet Denali: A machine learning potential for biological and organic chemistry with semi-empirical cost and DFT accuracy. Journal of Chemical Physics, 2021, 155, 204103.	3.0	40
15	Interactions between Methane and Polycyclic Aromatic Hydrocarbons: A High Accuracy Benchmark Study. Journal of Chemical Theory and Computation, 2013, 9, 370-389.	5.3	36
16	An accurate benchmark description of the interactions between carbon dioxide and polyheterocyclic aromatic compounds containing nitrogen. Physical Chemistry Chemical Physics, 2015, 17, 16560-16574.	2.8	30
17	Sharing Data from Molecular Simulations. Journal of Chemical Information and Modeling, 2019, 59, 4093-4099.	5.4	26
18	Toward an Accurate Description of Methane Physisorption on Carbon Nanotubes. Journal of Physical Chemistry C, 2014, 118, 544-550.	3.1	22

#	Article	IF	Citations
19	Driving torsion scans with wavefront propagation. Journal of Chemical Physics, 2020, 152, 244116.	3.0	22
20	The CECAM electronic structure library and the modular software development paradigm. Journal of Chemical Physics, 2020, 153, 024117.	3.0	19
21	Efficient and automated computation of accurate molecular geometries using focal-point approximations to large-basis coupled-cluster theory. Journal of Chemical Physics, 2020, 152, 124109.	3.0	15
22	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.	3.0	15
23	Highly Correlated Electronic Structure Calculations of the Heâ€“C₃â€¦â€¦ van der Waals Complex and Collision-Induced Rotational Transitions of C₃. Journal of Physical Chemistry A, 2014, 118, 6351-6360.	2.5	13
24	First-order symmetry-adapted perturbation theory for multiplet splittings. Journal of Chemical Physics, 2018, 148, 164110.	3.0	12
25	Stochastic resolution of identity second-order Matsubara Greenâ€™s function theory. Journal of Chemical Physics, 2019, 151, 044114.	3.0	9
26	Implementation of symmetry-adapted perturbation theory based on density functional theory and using hybrid exchangeâ€“correlation kernels for dispersion terms. Journal of Chemical Physics, 2022, 157, .	3.0	6
27	Optimized damping parameters for empirical dispersion corrections to symmetry-adapted perturbation theory. Journal of Chemical Physics, 2021, 154, 234107.	3.0	3