

Daniel G A Smith

List of Publications by Year in descending order

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27
papers

2,633
citations

394421

19
h-index

526287

27
g-index

34
all docs

34
docs citations

34
times ranked

3310
citing authors

#	ARTICLE	IF	CITATIONS
1	Implementation of symmetry-adapted perturbation theory based on density functional theory and using hybrid exchange–correlation kernels for dispersion terms. <i>Journal of Chemical Physics</i> , 2022, 157, .	3.0	6
2	The MolSSI QCArchive project: An open-source platform to compute, organize, and share quantum chemistry data. <i>Wiley Interdisciplinary Reviews: Computational Molecular Science</i> , 2021, 11, e1491.	14.6	42
3	Optimized damping parameters for empirical dispersion corrections to symmetry-adapted perturbation theory. <i>Journal of Chemical Physics</i> , 2021, 154, 234107.	3.0	3
4	Development and Benchmarking of Open Force Field v1.0.0—the Parsley Small-Molecule Force Field. <i>Journal of Chemical Theory and Computation</i> , 2021, 17, 6262-6280.	5.3	80
5	OrbNet Denali: A machine learning potential for biological and organic chemistry with semi-empirical cost and DFT accuracy. <i>Journal of Chemical Physics</i> , 2021, 155, 204103.	3.0	40
6	Quantum Chemistry Common Driver and Databases (QCDB) and Quantum Chemistry Engine (QCEngine): Automation and interoperability among computational chemistry programs. <i>Journal of Chemical Physics</i> , 2021, 155, 204801.	3.0	15
7	The CECAM electronic structure library and the modular software development paradigm. <i>Journal of Chemical Physics</i> , 2020, 153, 024117.	3.0	19
8	PSI4 1.4: Open-source software for high-throughput quantum chemistry. <i>Journal of Chemical Physics</i> , 2020, 152, 184108.	3.0	440
9	Efficient and automated computation of accurate molecular geometries using focal-point approximations to large-basis coupled-cluster theory. <i>Journal of Chemical Physics</i> , 2020, 152, 124109.	3.0	15
10	Driving torsion scans with wavefront propagation. <i>Journal of Chemical Physics</i> , 2020, 152, 244116.	3.0	22
11	Stochastic resolution of identity second-order Matsubara Green's function theory. <i>Journal of Chemical Physics</i> , 2019, 151, 044114.	3.0	9
12	Sharing Data from Molecular Simulations. <i>Journal of Chemical Information and Modeling</i> , 2019, 59, 4093-4099.	5.4	26
13	PES-Learn: An Open-Source Software Package for the Automated Generation of Machine Learning Models of Molecular Potential Energy Surfaces. <i>Journal of Chemical Theory and Computation</i> , 2019, 15, 4386-4398.	5.3	51
14	First-order symmetry-adapted perturbation theory for multiplet splittings. <i>Journal of Chemical Physics</i> , 2018, 148, 164110.	3.0	12
15	Perspective: Computational chemistry software and its advancement as illustrated through three grand challenge cases for molecular science. <i>Journal of Chemical Physics</i> , 2018, 149, 180901.	3.0	72
16	Psi4Numpy: An Interactive Quantum Chemistry Programming Environment for Reference Implementations and Rapid Development. <i>Journal of Chemical Theory and Computation</i> , 2018, 14, 3504-3511.	5.3	106
17	opt_einsum - A Python package for optimizing contraction order for einsum-like expressions. <i>Journal of Open Source Software</i> , 2018, 3, 753.	4.6	46
18	Psi4 1.1: An Open-Source Electronic Structure Program Emphasizing Automation, Advanced Libraries, and Interoperability. <i>Journal of Chemical Theory and Computation</i> , 2017, 13, 3185-3197.	5.3	961

#	ARTICLE	IF	CITATIONS
19	The BioFragment Database (BFDb): An open-data platform for computational chemistry analysis of noncovalent interactions. <i>Journal of Chemical Physics</i> , 2017, 147, 161727.	3.0	82
20	Revised Damping Parameters for the D3 Dispersion Correction to Density Functional Theory. <i>Journal of Physical Chemistry Letters</i> , 2016, 7, 2197-2203.	4.6	305
21	Benchmarking the CO ₂ Adsorption Energy on Carbon Nanotubes. <i>Journal of Physical Chemistry C</i> , 2015, 119, 4934-4948.	3.1	47
22	An accurate benchmark description of the interactions between carbon dioxide and polyheterocyclic aromatic compounds containing nitrogen. <i>Physical Chemistry Chemical Physics</i> , 2015, 17, 16560-16574.	2.8	30
23	Toward an Accurate Description of Methane Physisorption on Carbon Nanotubes. <i>Journal of Physical Chemistry C</i> , 2014, 118, 544-550.	3.1	22
24	Highly Correlated Electronic Structure Calculations of the He-C ₃ van der Waals Complex and Collision-Induced Rotational Transitions of C ₃ . <i>Journal of Physical Chemistry A</i> , 2014, 118, 6351-6360.	2.5	13
25	Basis Set Convergence of the Post-CCSD(T) Contribution to Noncovalent Interaction Energies. <i>Journal of Chemical Theory and Computation</i> , 2014, 10, 3140-3150.	5.3	43
26	Interactions between Methane and Polycyclic Aromatic Hydrocarbons: A High Accuracy Benchmark Study. <i>Journal of Chemical Theory and Computation</i> , 2013, 9, 370-389.	5.3	36
27	Highly accurate potential energy surface for the He-H ₂ dimer. <i>Journal of Chemical Physics</i> , 2013, 139, 144305.	3.0	46