Konrad Patkowski

List of Publications by Year
in descending order

57	4,174	159585 30	149698 56
papers	citations	h-index	g-index

60	60	60	3776
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	Dispersionless Density Functional Theory. Physical Review Letters, 2009, 103, 263201.	7.8	159
5	Intermolecular Interactions via Perturbation Theory: From Diatoms to Biomolecules. , 0, , 43-117.		145
6	Pair potential for helium from symmetry-adapted perturbation theory calculations and from supermolecular data. Journal of Chemical Physics, 2007, 127, 124303.	3.0	145
7	Argon pair potential at basis set and excitation limits. Journal of Chemical Physics, 2010, 133, 094304.	3.0	126
8	Potential energy surface for interactions between two hydrogen molecules. Journal of Chemical Physics, 2008, 129, 094304.	3.0	123
9	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
10	Accurateab initiopotential for argon dimer including highly repulsive region. Molecular Physics, 2005, 103, 2031-2045.	1.7	105
11	Improved interaction energy benchmarks for dimers of biological relevance. Physical Chemistry Chemical Physics, 2010, 12, 5974.	2.8	102
12	Recent developments in symmetryâ€adapted perturbation theory. Wiley Interdisciplinary Reviews: Computational Molecular Science, 2020, 10, e1452.	14.6	102
13	On the Elusive Twelfth Vibrational State of Beryllium Dimer. Science, 2009, 326, 1382-1384.	12.6	94
14	Third-order interactions in symmetry-adapted perturbation theory. Journal of Chemical Physics, 2006, 125, 154107.	3.0	93
15	Interactions in Diatomic Dimers Involving Closed-Shell Metals. Journal of Physical Chemistry A, 2007, 111, 12822-12838.	2.5	90
16	Extension of the Hartreeâ^'Fock Plus Dispersion Method by First-Order Correlation Effects. Journal of Physical Chemistry Letters, 2010, 1, 550-555.	4.6	83
17	Accurate Pair Interaction Energies for Helium from Supermolecular Gaussian Geminal Calculationsâ€. Journal of Physical Chemistry A, 2007, 111, 7611-7623.	2.5	55
18	Ab initio potential energy surface and second virial coefficient for Heâ€“H2O complex. Computational and Theoretical Chemistry, 2002, 591, 231-243.	1.5	54

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19	Full-configuration-interaction calculation of three-body nonadditive contribution to helium interaction potential. Journal of Chemical Physics, 2009, 131, 064105.	3.0	50
20	On the accuracy of explicitly correlated coupled-cluster interaction energies â€" have orbital results been beaten yet?. Journal of Chemical Physics, 2012, 137, 034103.	3.0	49
21	Benchmarking the CO₂ Adsorption Energy on Carbon Nanotubes. Journal of Physical Chemistry C, 2015, 119, 4934-4948.	3.1	47
22	Highly accurate potential energy surface for the Heâ€“H2 dimer. Journal of Chemical Physics, 2013, 139, 144305.	3.0	46
23	Unified treatment of chemical and van der Waals forces via symmetry-adapted perturbation expansion. Journal of Chemical Physics, 2004, 120, 6849-6862.	3.0	44
24	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
25	Rovibrational line-shape parameters for H2 in He and new H2-He potential energy surface. Journal of Quantitative Spectroscopy and Radiative Transfer, 2017, 202, 308-320.	2.3	42
26	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
27	Complete basis set extrapolations of dispersion, exchange, and coupledâ€clusters contributions to the interaction energy: a helium dimer study. International Journal of Quantum Chemistry, 2008, 108, 2053-2075.	2.0	35
28	Accurate ab initio potential for the krypton dimer and transport properties of the low-density krypton gas. Journal of Chemical Physics, 2015, 142, 204307.	3.0	33
29	Platinum, gold, and silver standards of intermolecular interaction energy calculations. Journal of Chemical Physics, 2019, 151, 070901.	3.0	33
30	Convergence behavior of the symmetry-adapted perturbation theory for states submerged in Pauli forbidden continuum. Journal of Chemical Physics, 2001, 115, 1137-1152.	3.0	32
31	Orbital relaxation and the third-order induction energy in symmetry-adapted perturbation theory. Theoretical Chemistry Accounts, 2010, 127, 211-221.	1.4	30
32	Basis set converged weak interaction energies from conventional and explicitly correlated coupled-cluster approach. Journal of Chemical Physics, 2013, 138, 154101.	3.0	30
33	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
34	Symmetry-adapted perturbation theory with regularized Coulomb potential. Computational and Theoretical Chemistry, 2001, 547, 293-307.	1.5	26
35	Frozen core and effective core potentials in symmetry-adapted perturbation theory. Journal of Chemical Physics, 2007, 127, 164103.	3.0	26
36	Elastic and rotationally inelastic differential cross sections for He+H2O collisions. Journal of Chemical Physics, 2002, 117, 11166-11174.	3.0	25

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37	Symmetry-forcing procedure and convergence behavior of perturbation expansions for molecular interaction energies. Journal of Chemical Physics, 2002, 117, 5124-5134.	3.0	24
38	H2 -He collisions: Ab initio theory meets cavity-enhanced spectra. Physical Review A, 2020, 101, .	2.5	24
39	Toward an Accurate Description of Methane Physisorption on Carbon Nanotubes. Journal of Physical Chemistry C, 2014, 118, 544-550.	3.1	22
40	Improving â€œSilver-Standardâ€•Benchmark Interaction Energies with Bond Functions. Journal of Chemical Theory and Computation, 2018, 14, 3053-3070.	5.3	16
41	Convergence Behavior of Symmetry-Adapted Perturbation Expansions for Excited States. A Model Study of Interactions Involving a Triplet Helium Atom. Collection of Czechoslovak Chemical Communications, 2004, 69, 141-176.	1.0	14
42	Portable parallel implementation of symmetry-adapted perturbation theory code. Molecular Physics, 2006, 104, 2241-2262.	1.7	13
43	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
44	Explicitly Correlated Dispersion and Exchange Dispersion Energies in Symmetry-Adapted Perturbation Theory. Journal of Chemical Theory and Computation, 2019, 15, 5965-5986.	5.3	13
45	First-order symmetry-adapted perturbation theory for multiplet splittings. Journal of Chemical Physics, 2018, 148, 164110.	3.0	12
46	Fully Quantum Cross Second Virial Coefficients for the Three-Dimensional Heâ€“H $$_{2}$$ 2 Pair. International Journal of Thermophysics, 2014, 35, 1435-1449.	2.1	10
47	Spin splittings from first-order symmetry-adapted perturbation theory without single-exchange approximation. Journal of Chemical Physics, 2019, 150, 074109.	3.0	9
48	Benchmark Databases of Intermolecular Interaction Energies: Design, Construction, and Significance. Annual Reports in Computational Chemistry, 2017, 13, 3-91.	1.7	8
49	Collisional line-shape effects in accurate He-perturbed H<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" altimg="si1.svg"><mml:msub><mml:mrow /><mml:mn>2</mml:mn></mml:msub></mml:math> spectra. Journal of Quantitative Spectroscopy and Radiative Transfer, 2022, 277, 107951.	2.3	8
50	Nonapproximated third-order exchange induction energy in symmetry-adapted perturbation theory. Journal of Chemical Physics, 2021, 154, 024103.	3.0	7
51	Efficient Density-Fitted Explicitly Correlated Dispersion and Exchange Dispersion Energies. Journal of Chemical Theory and Computation, 2021, 17, 1435-1456.	5.3	5
52	Accurate virial coefficients of gaseous krypton from state-of-the-art ab initio potential and polarizability of the krypton dimer. Journal of Chemical Physics, 2018, 148, 024306.	3.0	4
53	Chiral Self Recognition: Interactions in Propylene Oxide Complexes. Journal of Physical Chemistry A, 2019, 123, 8607-8618.	2.5	4
54	Ab Initio Study of Chiral Discrimination in the Glycidol Dimer. Journal of Physical Chemistry A, 2020, 124, 9436-9450.	2.5	3

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55	Extension of an Atomâ€“Atom Dispersion Function to Halogen Bonds and Its Use for Rational Design of Drugs and Biocatalysts. Journal of Physical Chemistry A, 2021, 125, 1787-1799.	2.5	3
56	Heats of formation and thermal stability of substituted 1,1â€²â€²Azobis(tetrazole) compounds with an extended nitrogen chain. International Journal of Quantum Chemistry, 2019, 119, e25794.	2.0	2
57	Interactions of CO₂ with cluster models of <scp>metalâ€“organic</scp> frameworks. Journal of Computational Chemistry, 2020, 41, 2066-2083.	3.3	0