Andreas Hansen

List of Publications by Year
in descending order

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Version: 2024-02-01

53 papers	8,918 citations	136950 32 h-index	168389 53 g-index
55 all docs	55 docs citations	55 times ranked	7070 citing authors

#	Article	IF	Citations
1	Natural triple excitations in local coupled cluster calculations with pair natural orbitals. Journal of Chemical Physics, 2013, 139, 134101.	3.0	1,240
2	A look at the density functional theory zoo with the advanced GMTKN55 database for general main group thermochemistry, kinetics and noncovalent interactions. Physical Chemistry Chemical Physics, 2017, 19, 32184-32215.	2.8	1,230
3	Dispersion-Corrected Mean-Field Electronic Structure Methods. Chemical Reviews, 2016, 116, 5105-5154.	47.7	1,032
4	A generally applicable atomic-charge dependent London dispersion correction. Journal of Chemical Physics, 2019, 150, 154122.	3.0	697
5	Consistent structures and interactions by density functional theory with small atomic orbital basis sets. Journal of Chemical Physics, 2015, 143, 054107.	3.0	605
6	Extended <scp>tightâ€binding</scp> quantum chemistry methods. Wiley Interdisciplinary Reviews: Computational Molecular Science, 2021, 11, e1493.	14.6	596
7	Efficient and accurate approximations to the local coupled cluster singles doubles method using a truncated pair natural orbital basis. Journal of Chemical Physics, 2009, 131, 064103.	3.0	468
8	B97-3c: A revised low-cost variant of the B97-D density functional method. Journal of Chemical Physics, 2018, 148, 064104.	3.0	400
9	r2SCAN-3c: A â€œSwiss army knifeâ€•composite electronic-structure method. Journal of Chemical Physics, 2021, 154, 064103.	3.0	290
10	Comprehensive Thermochemical Benchmark Set of Realistic Closed-Shell Metal Organic Reactions. Journal of Chemical Theory and Computation, 2018, 14, 2596-2608.	5.3	202
11	A Practicable Realâ€Space Measure and Visualization of Static Electronâ€Correlation Effects. Angewandte Chemie - International Edition, 2015, 54, 12308-12313.	13.8	194
12	Efficient and accurate local single reference correlation methods for high-spin open-shell molecules using pair natural orbitals. Journal of Chemical Physics, 2011, 135, 214102.	3.0	165
13	Fully Automated Quantumâ€Chemistryâ€Based Computation of Spinâ€“Spinâ€Coupled Nuclear Magnetic Resonance Spectra. Angewandte Chemie - International Edition, 2017, 56, 14763-14769.	13.8	158
14	Understanding and Quantifying London Dispersion Effects in Organometallic Complexes. Accounts of Chemical Research, 2019, 52, 258-266.	15.6	117
15	Efficient Quantum Chemical Calculation of Structure Ensembles and Free Energies for Nonrigid Molecules. Journal of Physical Chemistry A, 2021, 125, 4039-4054.	2.5	105
16	The Fractional Occupation Number Weighted Density as a Versatile Analysis Tool for Molecules with a Complicated Electronic Structure. Chemistry - A European Journal, 2017, 23, 6150-6164.	3.3	102
17	Quantum Chemical Benchmark Study on 46 RNA Backbone Families Using a Dinucleotide Unit. Journal of Chemical Theory and Computation, 2015, 11, 4972-4991.	5.3	90
18	Hydrosilylation of Ketones, Imines and Nitriles Catalysed by Electrophilic Phosphonium Cations: Functional Group Selectivity and Mechanistic Considerations. Chemistry - A European Journal, 2015, 21, 6491-6500.	3.3	78

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19	The Thermochemistry of London Dispersionâ€Driven Transition Metal Reactions: Getting the â€˜Right Answer for the Right Reasonâ€™. ChemistryOpen, 2014, 3, 177-189.	1.9	77
20	Assessing Density Functional Theory for Chemically Relevant Open-Shell Transition Metal Reactions. Journal of Chemical Theory and Computation, 2021, 17, 6134-6151.	5.3	75
21	A diuranium carbide cluster stabilized inside a C80 fullerene cage. Nature Communications, 2018, 9, 2753.	12.8	63
22	HYDROPHOBE Challenge: A Joint Experimental and Computational Study on the Hostâ€“Guest Binding of Hydrocarbons to Cucurbiturils, Allowing Explicit Evaluation of Guest Hydration Free-Energy Contributions. Journal of Physical Chemistry B, 2017, 121, 11144-11162.	2.6	62
23	Semiautomated Transition State Localization for Organometallic Complexes with Semiempirical Quantum Chemical Methods. Journal of Chemical Theory and Computation, 2020, 16, 2002-2012.	5.3	60
24	Comprehensive theoretical study of all 1812 C₆₀ isomers. Physical Chemistry Chemical Physics, 2017, 19, 14296-14305.	2.8	58
25	A general intermolecular force field based on tight-binding quantum chemical calculations. Journal of Chemical Physics, 2017, 147, 161708.	3.0	53
26	Theoretical study on conformational energies of transition metal complexes. Physical Chemistry Chemical Physics, 2021, 23, 287-299.	2.8	52
27	Benchmark Study of Electrochemical Redox Potentials Calculated with Semiempirical and DFT Methods. Journal of Physical Chemistry A, 2020, 124, 7166-7176.	2.5	45
28	Automated Molecular Cluster Growing for Explicit Solvation by Efficient Force Field and Tight Binding Methods. Journal of Chemical Theory and Computation, 2022, 18, 3174-3189.	5.3	45
29	The furan microsolvation blind challenge for quantum chemical methods: First steps. Journal of Chemical Physics, 2018, 148, 014301.	3.0	44
30	Fast and Reasonable Geometry Optimization of Lanthanoid Complexes with an Extended Tight Binding Quantum Chemical Method. Inorganic Chemistry, 2017, 56, 12485-12491.	4.0	41
31	Evidence of a Donorâ€“Acceptor (Irâ€“H)â†’SiR₃ Interaction in a Trapped Ir(III) Silane Catalytic Intermediate. Organometallics, 2016, 35, 2207-2223.	2.3	40
32	Finding the best density functional approximation to describe interaction energies and structures of ionic liquids in molecular dynamics studies. Journal of Chemical Physics, 2018, 148, 193835.	3.0	38
33	Coâ€“C Bond Dissociation Energies in Cobalamin Derivatives and Dispersion Effects: Anomaly or Just Challenging?. Journal of Chemical Theory and Computation, 2015, 11, 1037-1045.	5.3	34
34	Quantum Chemical Calculation of Molecular and Periodic Peptide and Protein Structures. Journal of Physical Chemistry B, 2020, 124, 3636-3646.	2.6	33
35	Vollautomatisierte quantenchemische Berechnung von Spinâ€Spinâ€gekoppelten magnetischen Kernspinresonanzspektren. Angewandte Chemie, 2017, 129, 14958-14964.	2.0	32
36	Benchmarking London dispersion corrected density functional theory for noncovalent ionâ€“Ï€ interactions. Physical Chemistry Chemical Physics, 2021, 23, 11635-11648.	2.8	31

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37	The first microsolvation step for furans: New experiments and benchmarking strategies. Journal of Chemical Physics, 2020, 152, 164303.	3.0	28
38	TEMPO-Mediated Catalysis of the Sterically Hindered Hydrogen Atom Transfer Reaction between (C₅Ph₅)Cr(CO)₃H and a Trityl Radical. Journal of the American Chemical Society, 2019, 141, 1882-1886.	13.7	25
39	Quantification of Noncovalent Interactions in Azideâ€“Pnictogen, â€“Chalcogen, and â€“Halogen Contacts. Chemistry - A European Journal, 2021, 27, 4627-4639.	3.3	25
40	The Association of Two â€œFrustratedâ€•Lewis Pairs by Stateâ€•ofâ€theâ€Art Quantum Chemical Methods. Israel Journal of Chemistry, 2015, 55, 235-242.	2.3	23
41	PCM-ROKS for the Description of Charge-Transfer States in Solution: Singletâ€“Triplet Gaps with Chemical Accuracy from Open-Shell Kohnâ€“Sham Reaction-Field Calculations. Journal of Physical Chemistry Letters, 2021, 12, 8470-8480.	4.6	23
42	[Cl@Si₂₀H₂₀]^{â^'}: Parent Siladodecahedrane with Endohedral Chloride Ion. Journal of the American Chemical Society, 2021, 143, 10865-10871.	13.7	20
43	Donorâ€“acceptor interactions between cyclic trinuclear pyridinate gold(<scp>i</scp>)-complexes and electron-poor guests: nature and energetics of guest-binding and templating on graphite. Chemical Science, 2018, 9, 3477-3483.	7.4	19
44	Accurate Thermochemistry for Large Molecules with Modern Density Functionals. Topics in Current Chemistry, 2014, , 1-23.	4.0	17
45	Conformational Energy Benchmark for Longer n-Alkane Chains. Journal of Physical Chemistry A, 2022, 126, 3521-3535.	2.5	16
46	Towards understanding solvation effects on the conformational entropy of non-rigid molecules. Physical Chemistry Chemical Physics, 2022, 24, 12249-12259.	2.8	15
47	Thermodynamics of H⁺/H^{â€¢}/H^{â€“}/e^{â€“} Transfer from [CpV(CO)₃H]^{â^'}: Comparisons to the Isoelectronic CpCr(CO)₃H. Organometallics, 2019, 38, 4319-4328.	2.3	10
48	transâ€“cis Câ€“Pdâ€“C rearrangement in hemichelates. Dalton Transactions, 2017, 46, 8125-8137.	3.3	9
49	Comment on â€œThe Nature of Chalcogenâ€Bondingâ€Type Telluriumâ€“Nitrogen Interactionsâ€• Fixing the Description of Finiteâ€Temperature Effects Restores the Agreement Between Experiment and Theory. Angewandte Chemie - International Edition, 2021, 60, 13144-13149.	13.8	8
50	Ligand Protonation at Carbon, not Nitrogen, during H₂ Production with Amine-Rich Iron Electrocatalysts. Inorganic Chemistry, 2021, 60, 17407-17413.	4.0	6
51	Hydrogen atom transfer rates from Tp-containing metal-hydrides to trityl radicals. Canadian Journal of Chemistry, 2021, 99, 216-220.	1.1	5
52	Comment on â€œThe Nature of Chalcogenâ€Bondingâ€Type Telluriumâ€“Nitrogen Interactionsâ€• Fixing the Description of Finiteâ€Temperature Effects Restores the Agreement Between Experiment and Theory. Angewandte Chemie, 2021, 133, 13252-13257.	2.0	4
53	Computational study of groundâ€state properties of Î¼ ₂ â€bridged group 14 porphyrinic sandwich complexes. Journal of Computational Chemistry, 2022, , .	3.3	1