Andreas Hansen

List of Publications by Year
in descending order

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53	8,918	136740	168136
papers	citations	32 h-index	53 g-index

55	55	55	7070
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	Computational study of groundâ€state properties of Î¼ ₂ â€bridged group 14 porphyrinic sandwich complexes. Journal of Computational Chemistry, 2022, , .	1.5	1
2	Towards understanding solvation effects on the conformational entropy of non-rigid molecules. Physical Chemistry Chemical Physics, 2022, 24, 12249-12259.	1.3	15
3	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.	2.3	45
4	Conformational Energy Benchmark for Longer n-Alkane Chains. Journal of Physical Chemistry A, 2022, 126, 3521-3535.	1.1	16
5	Extended <scp>tightâ€binding</scp> quantum chemistry methods. Wiley Interdisciplinary Reviews: Computational Molecular Science, 2021, 11, e1493.	6.2	596
6	Quantification of Noncovalent Interactions in Azideâ€“Pnictogen, â€“Chalcogen, and â€“Halogen Contacts. Chemistry - A European Journal, 2021, 27, 4627-4639.	1.7	25
7	Theoretical study on conformational energies of transition metal complexes. Physical Chemistry Chemical Physics, 2021, 23, 287-299.	1.3	52
8	Benchmarking London dispersion corrected density functional theory for noncovalent ionâ€“Ï€ interactions. Physical Chemistry Chemical Physics, 2021, 23, 11635-11648.	1.3	31
9	r2SCAN-3c: A â€œSwiss army knifeâ€•composite electronic-structure method. Journal of Chemical Physics, 2021, 154, 064103.	1.2	290
10	Efficient Quantum Chemical Calculation of Structure Ensembles and Free Energies for Nonrigid Molecules. Journal of Physical Chemistry A, 2021, 125, 4039-4054.	1.1	105
11	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.	1.6	4
12	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.	7.2	8
13	[Cl@Si₂₀H₂₀]^{â^'}: Parent Siladodecahedrane with Endohedral Chloride Ion. Journal of the American Chemical Society, 2021, 143, 10865-10871.	6.6	20
14	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.	2.1	23
15	Assessing Density Functional Theory for Chemically Relevant Open-Shell Transition Metal Reactions. Journal of Chemical Theory and Computation, 2021, 17, 6134-6151.	2.3	75
16	Hydrogen atom transfer rates from Tp-containing metal-hydrides to trityl radicals. Canadian Journal of Chemistry, 2021, 99, 216-220.	0.6	5
17	Ligand Protonation at Carbon, not Nitrogen, during H₂ Production with Amine-Rich Iron Electrocatalysts. Inorganic Chemistry, 2021, 60, 17407-17413.	1.9	6
18	Benchmark Study of Electrochemical Redox Potentials Calculated with Semiempirical and DFT Methods. Journal of Physical Chemistry A, 2020, 124, 7166-7176.	1.1	45

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19	The first microsolvation step for furans: New experiments and benchmarking strategies. Journal of Chemical Physics, 2020, 152, 164303.	1.2	28
20	Semiautomated Transition State Localization for Organometallic Complexes with Semiempirical Quantum Chemical Methods. Journal of Chemical Theory and Computation, 2020, 16, 2002-2012.	2.3	60
21	Quantum Chemical Calculation of Molecular and Periodic Peptide and Protein Structures. Journal of Physical Chemistry B, 2020, 124, 3636-3646.	1.2	33
22	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.	1.1	10
23	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.	6.6	25
24	A generally applicable atomic-charge dependent London dispersion correction. Journal of Chemical Physics, 2019, 150, 154122.	1.2	697
25	Understanding and Quantifying London Dispersion Effects in Organometallic Complexes. Accounts of Chemical Research, 2019, 52, 258-266.	7.6	117
26	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.	1.2	38
27	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.	3.7	19
28	B97-3c: A revised low-cost variant of the B97-D density functional method. Journal of Chemical Physics, 2018, 148, 064104.	1.2	400
29	The furan microsolvation blind challenge for quantum chemical methods: First steps. Journal of Chemical Physics, 2018, 148, 014301.	1.2	44
30	Comprehensive Thermochemical Benchmark Set of Realistic Closed-Shell Metal Organic Reactions. Journal of Chemical Theory and Computation, 2018, 14, 2596-2608.	2.3	202
31	A diuranium carbide cluster stabilized inside a C80 fullerene cage. Nature Communications, 2018, 9, 2753.	5.8	63
32	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.	1.7	102
33	Comprehensive theoretical study of all 1812 C₆₀ isomers. Physical Chemistry Chemical Physics, 2017, 19, 14296-14305.	1.3	58
34	transâ€“cis Câ€“Pdâ€“C rearrangement in hemichelates. Dalton Transactions, 2017, 46, 8125-8137.	1.6	9
35	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.	1.3	1,230
36	Fast and Reasonable Geometry Optimization of Lanthanoid Complexes with an Extended Tight Binding Quantum Chemical Method. Inorganic Chemistry, 2017, 56, 12485-12491.	1.9	41

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37	Vollautomatisierte quantenchemische Berechnung von Spinâ€Spinâ€gekoppelten magnetischen Kernspinresonanzspektren. Angewandte Chemie, 2017, 129, 14958-14964.	1.6	32
38	Fully Automated Quantumâ€Chemistryâ€Based Computation of Spinâ€“Spinâ€Coupled Nuclear Magnetic Resonance Spectra. Angewandte Chemie - International Edition, 2017, 56, 14763-14769.	7.2	158
39	A general intermolecular force field based on tight-binding quantum chemical calculations. Journal of Chemical Physics, 2017, 147, 161708.	1.2	53
40	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.	1.2	62
41	Dispersion-Corrected Mean-Field Electronic Structure Methods. Chemical Reviews, 2016, 116, 5105-5154.	23.0	1,032
42	Evidence of a Donorâ€“Acceptor (Irâ€“H)â†'SiR₃ Interaction in a Trapped Ir(III) Silane Catalytic Intermediate. Organometallics, 2016, 35, 2207-2223.	1.1	40
43	The Association of Two â€œFrustratedâ€•Lewis Pairs by Stateâ€ofâ€theâ€Art Quantum Chemical Methods. Israel Journal of Chemistry, 2015, 55, 235-242.	1.0	23
44	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.	2.3	34
45	A Practicable Realâ€Space Measure and Visualization of Static Electronâ€Correlation Effects. Angewandte Chemie - International Edition, 2015, 54, 12308-12313.	7.2	194
46	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.	1.7	78
47	Consistent structures and interactions by density functional theory with small atomic orbital basis sets. Journal of Chemical Physics, 2015, 143, 054107.	1.2	605
48	Quantum Chemical Benchmark Study on 46 RNA Backbone Families Using a Dinucleotide Unit. Journal of Chemical Theory and Computation, 2015, 11, 4972-4991.	2.3	90
49	Accurate Thermochemistry for Large Molecules with Modern Density Functionals. Topics in Current Chemistry, 2014, , 1-23.	4.0	17
50	The Thermochemistry of London Dispersionâ€Driven Transition Metal Reactions: Getting the â€˜Right Answer for the Right Reasonâ€™. ChemistryOpen, 2014, 3, 177-189.	0.9	77
51	Natural triple excitations in local coupled cluster calculations with pair natural orbitals. Journal of Chemical Physics, 2013, 139, 134101.	1.2	1,240
52	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.	1.2	165
53	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.	1.2	468