

Andreas Hansen

List of Publications by Year in descending order

Source: <https://exaly.com/author-pdf/7975567/publications.pdf>

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	Computational study of ground-state properties of μ_2 -bridged group 14 porphyrinic sandwich complexes. <i>Journal of Computational Chemistry</i> , 2022, , .	3.3	1
2	Towards understanding solvation effects on the conformational entropy of non-rigid molecules. <i>Physical Chemistry Chemical Physics</i> , 2022, 24, 12249-12259.	2.8	15
3	Automated Molecular Cluster Growing for Explicit Solvation by Efficient Force Field and Tight Binding Methods. <i>Journal of Chemical Theory and Computation</i> , 2022, 18, 3174-3189.	5.3	45
4	Conformational Energy Benchmark for Longer n -Alkane Chains. <i>Journal of Physical Chemistry A</i> , 2022, 126, 3521-3535.	2.5	16
5	Extended tight-binding quantum chemistry methods. <i>Wiley Interdisciplinary Reviews: Computational Molecular Science</i> , 2021, 11, e1493.	14.6	596
6	Quantification of Noncovalent Interactions in Azide-Pnictogen, Chalcogen, and Halogen Contacts. <i>Chemistry - A European Journal</i> , 2021, 27, 4627-4639.	3.3	25
7	Theoretical study on conformational energies of transition metal complexes. <i>Physical Chemistry Chemical Physics</i> , 2021, 23, 287-299.	2.8	52
8	Benchmarking London dispersion corrected density functional theory for noncovalent ion interactions. <i>Physical Chemistry Chemical Physics</i> , 2021, 23, 11635-11648.	2.8	31
9	r2SCAN-3c: A Swiss army knife-composite electronic-structure method. <i>Journal of Chemical Physics</i> , 2021, 154, 064103.	3.0	290
10	Efficient Quantum Chemical Calculation of Structure Ensembles and Free Energies for Nonrigid Molecules. <i>Journal of Physical Chemistry A</i> , 2021, 125, 4039-4054.	2.5	105
11	Comment on "The Nature of Chalcogen-Bonding-Type Tellurium-Nitrogen Interactions": Fixing the Description of Finite-Temperature Effects Restores the Agreement Between Experiment and Theory. <i>Angewandte Chemie</i> , 2021, 133, 13252-13257.	2.0	4
12	Comment on "The Nature of Chalcogen-Bonding-Type Tellurium-Nitrogen Interactions": Fixing the Description of Finite-Temperature Effects Restores the Agreement Between Experiment and Theory. <i>Angewandte Chemie - International Edition</i> , 2021, 60, 13144-13149.	13.8	8
13	$[\text{Cl@Si}_{20}\text{H}_{20}]^+$: Parent Siladodecahedrane with Endohedral Chloride Ion. <i>Journal of the American Chemical Society</i> , 2021, 143, 10865-10871.	13.7	20
14	PCM-ROKS for the Description of Charge-Transfer States in Solution: Singlet-Triplet Gaps with Chemical Accuracy from Open-Shell Kohn-Sham Reaction-Field Calculations. <i>Journal of Physical Chemistry Letters</i> , 2021, 12, 8470-8480.	4.6	23
15	Assessing Density Functional Theory for Chemically Relevant Open-Shell Transition Metal Reactions. <i>Journal of Chemical Theory and Computation</i> , 2021, 17, 6134-6151.	5.3	75
16	Hydrogen atom transfer rates from Tp-containing metal-hydrides to trityl radicals. <i>Canadian Journal of Chemistry</i> , 2021, 99, 216-220.	1.1	5
17	Ligand Protonation at Carbon, not Nitrogen, during H_2 Production with Amine-Rich Iron Electrocatalysts. <i>Inorganic Chemistry</i> , 2021, 60, 17407-17413.	4.0	6
18	Benchmark Study of Electrochemical Redox Potentials Calculated with Semiempirical and DFT Methods. <i>Journal of Physical Chemistry A</i> , 2020, 124, 7166-7176.	2.5	45

#	ARTICLE	IF	CITATIONS
19	The first microsolvation step for furans: New experiments and benchmarking strategies. <i>Journal of Chemical Physics</i> , 2020, 152, 164303.	3.0	28
20	Semiautomated Transition State Localization for Organometallic Complexes with Semiempirical Quantum Chemical Methods. <i>Journal of Chemical Theory and Computation</i> , 2020, 16, 2002-2012.	5.3	60
21	Quantum Chemical Calculation of Molecular and Periodic Peptide and Protein Structures. <i>Journal of Physical Chemistry B</i> , 2020, 124, 3636-3646.	2.6	33
22	Thermodynamics of $H^+ / H^{\bullet} / H^{\ominus} / e^-$ Transfer from $[CpV(CO)_3H]^+$: Comparisons to the Isoelectronic $CpCr(CO)_3H$. <i>Organometallics</i> , 2019, 38, 4319-4328.	2.3	10
23	TEMPO-Mediated Catalysis of the Sterically Hindered Hydrogen Atom Transfer Reaction between $(C_5Ph_5)Cr(CO)_3H$ and a Trityl Radical. <i>Journal of the American Chemical Society</i> , 2019, 141, 1882-1886.	13.7	25
24	A generally applicable atomic-charge dependent London dispersion correction. <i>Journal of Chemical Physics</i> , 2019, 150, 154122.	3.0	697
25	Understanding and Quantifying London Dispersion Effects in Organometallic Complexes. <i>Accounts of Chemical Research</i> , 2019, 52, 258-266.	15.6	117
26	Finding the best density functional approximation to describe interaction energies and structures of ionic liquids in molecular dynamics studies. <i>Journal of Chemical Physics</i> , 2018, 148, 193835.	3.0	38
27	Donor-acceptor interactions between cyclic trinuclear pyridinate gold(<i>i</i>)-complexes and electron-poor guests: nature and energetics of guest-binding and templating on graphite. <i>Chemical Science</i> , 2018, 9, 3477-3483.	7.4	19
28	B97-3c: A revised low-cost variant of the B97-D density functional method. <i>Journal of Chemical Physics</i> , 2018, 148, 064104.	3.0	400
29	The furan microsolvation blind challenge for quantum chemical methods: First steps. <i>Journal of Chemical Physics</i> , 2018, 148, 014301.	3.0	44
30	Comprehensive Thermochemical Benchmark Set of Realistic Closed-Shell Metal Organic Reactions. <i>Journal of Chemical Theory and Computation</i> , 2018, 14, 2596-2608.	5.3	202
31	A diuranium carbide cluster stabilized inside a C80 fullerene cage. <i>Nature Communications</i> , 2018, 9, 2753.	12.8	63
32	The Fractional Occupation Number Weighted Density as a Versatile Analysis Tool for Molecules with a Complicated Electronic Structure. <i>Chemistry - A European Journal</i> , 2017, 23, 6150-6164.	3.3	102
33	Comprehensive theoretical study of all 1812 C_{60} isomers. <i>Physical Chemistry Chemical Physics</i> , 2017, 19, 14296-14305.	2.8	58
34	trans-cis Pd-C rearrangement in hemichelates. <i>Dalton Transactions</i> , 2017, 46, 8125-8137.	3.3	9
35	A look at the density functional theory zoo with the advanced GMTKN55 database for general main group thermochemistry, kinetics and noncovalent interactions. <i>Physical Chemistry Chemical Physics</i> , 2017, 19, 32184-32215.	2.8	1,230
36	Fast and Reasonable Geometry Optimization of Lanthanoid Complexes with an Extended Tight Binding Quantum Chemical Method. <i>Inorganic Chemistry</i> , 2017, 56, 12485-12491.	4.0	41

#	ARTICLE	IF	CITATIONS
37	Vollautomatisierte quantenchemische Berechnung von Spin-Spin-gekoppelten magnetischen Kernspinresonanzspektren. <i>Angewandte Chemie</i> , 2017, 129, 14958-14964.	2.0	32
38	Fully Automated Quantum-Chemistry-Based Computation of Spin-Spin-Coupled Nuclear Magnetic Resonance Spectra. <i>Angewandte Chemie - International Edition</i> , 2017, 56, 14763-14769.	13.8	158
39	A general intermolecular force field based on tight-binding quantum chemical calculations. <i>Journal of Chemical Physics</i> , 2017, 147, 161708.	3.0	53
40	HYDROPHOBE Challenge: A Joint Experimental and Computational Study on the Host-Guest Binding of Hydrocarbons to Cucurbiturils, Allowing Explicit Evaluation of Guest Hydration Free-Energy Contributions. <i>Journal of Physical Chemistry B</i> , 2017, 121, 11144-11162.	2.6	62
41	Dispersion-Corrected Mean-Field Electronic Structure Methods. <i>Chemical Reviews</i> , 2016, 116, 5105-5154.	47.7	1,032
42	Evidence of a Donor-Acceptor (Ir ^{III}) ₃ Interaction in a Trapped Ir(III) Silane Catalytic Intermediate. <i>Organometallics</i> , 2016, 35, 2207-2223.	2.3	40
43	The Association of Two Frustrated Lewis Pairs by State-of-the-Art Quantum Chemical Methods. <i>Israel Journal of Chemistry</i> , 2015, 55, 235-242.	2.3	23
44	Co-C Bond Dissociation Energies in Cobalamin Derivatives and Dispersion Effects: Anomaly or Just Challenging?. <i>Journal of Chemical Theory and Computation</i> , 2015, 11, 1037-1045.	5.3	34
45	A Practicable Real-Space Measure and Visualization of Static Electron-Correlation Effects. <i>Angewandte Chemie - International Edition</i> , 2015, 54, 12308-12313.	13.8	194
46	Hydrosilylation of Ketones, Imines and Nitriles Catalysed by Electrophilic Phosphonium Cations: Functional Group Selectivity and Mechanistic Considerations. <i>Chemistry - A European Journal</i> , 2015, 21, 6491-6500.	3.3	78
47	Consistent structures and interactions by density functional theory with small atomic orbital basis sets. <i>Journal of Chemical Physics</i> , 2015, 143, 054107.	3.0	605
48	Quantum Chemical Benchmark Study on 46 RNA Backbone Families Using a Dinucleotide Unit. <i>Journal of Chemical Theory and Computation</i> , 2015, 11, 4972-4991.	5.3	90
49	Accurate Thermochemistry for Large Molecules with Modern Density Functionals. <i>Topics in Current Chemistry</i> , 2014, , 1-23.	4.0	17
50	The Thermochemistry of London Dispersion-Driven Transition Metal Reactions: Getting the Right Answer for the Right Reason™. <i>ChemistryOpen</i> , 2014, 3, 177-189.	1.9	77
51	Natural triple excitations in local coupled cluster calculations with pair natural orbitals. <i>Journal of Chemical Physics</i> , 2013, 139, 134101.	3.0	1,240
52	Efficient and accurate local single reference correlation methods for high-spin open-shell molecules using pair natural orbitals. <i>Journal of Chemical Physics</i> , 2011, 135, 214102.	3.0	165
53	Efficient and accurate approximations to the local coupled cluster singles doubles method using a truncated pair natural orbital basis. <i>Journal of Chemical Physics</i> , 2009, 131, 064103.	3.0	468