Alexander A Auer

List of Publications by Year
in descending order

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48 papers	2,259 citations	236925 25 h-index	214800 47 g-index
50 all docs	50 docs citations	50 times ranked	2443 citing authors

#	Article	IF	Citations
1	Automatic Generation of Auxiliary Basis Sets. Journal of Chemical Theory and Computation, 2017, 13, 554-562.	5.3	384
2	Quantitative prediction of gas-phase 13C nuclear magnetic shielding constants. Journal of Chemical Physics, 2003, 118, 10407-10417.	3.0	246
3	Decomposition of Intermolecular Interaction Energies within the Local Pair Natural Orbital Coupled Cluster Framework. Journal of Chemical Theory and Computation, 2016, 12, 4778-4792.	5.3	231
4	A Supported Bismuth Halide Perovskite Photocatalyst for Selective Aliphatic and Aromatic Câ€“H Bond Activation. Angewandte Chemie - International Edition, 2020, 59, 5788-5796.	13.8	160
5	Understanding the Role of Dispersion in Frustrated Lewis Pairs and Classical Lewis Adducts: A Domainâ€Based Local Pair Natural Orbital Coupled Cluster Study. Chemistry - A European Journal, 2017, 23, 865-873.	3.3	91
6	Quantitative prediction of gas-phase F19 nuclear magnetic shielding constants. Journal of Chemical Physics, 2008, 128, 244111.	3.0	79
7	Efficient and Accurate Prediction of Nuclear Magnetic Resonance Shielding Tensors with Double-Hybrid Density Functional Theory. Journal of Chemical Theory and Computation, 2018, 14, 4756-4771.	5.3	75
8	Standardized Benchmarking of Water Splitting Catalysts in a Combined Electrochemical Flow Cell/Inductively Coupled Plasmaâ€“Optical Emission Spectrometry (ICP-OES) Setup. ACS Catalysis, 2017, 7, 3768-3778.	11.2	73
9	Self-Consistent Field Calculation of Nuclear Magnetic Resonance Chemical Shielding Constants Using Gauge-Including Atomic Orbitals and Approximate Two-Electron Integrals. Journal of Chemical Theory and Computation, 2018, 14, 619-637.	5.3	70
10	Nanocomposites with Structure Domains of 0.5 to 3â€…nm by Polymerization of Silicon Spiro Compounds. Angewandte Chemie - International Edition, 2009, 48, 8254-8258.	13.8	63
11	Bismuthâ€Arene Ï€-Interaction: A Combined Experimental and Theoretical Approach. Organometallics, 2009, 28, 5405-5411.	2.3	58
12	Treating Subvalence Correlation Effects in Domain Based Pair Natural Orbital Coupled Cluster Calculations: An Out-of-the-Box Approach. Journal of Chemical Theory and Computation, 2017, 13, 3220-3227.	5.3	45
13	The furan microsolvation blind challenge for quantum chemical methods: First steps. Journal of Chemical Physics, 2018, 148, 014301.	3.0	44
14	Pair natural orbital and canonical coupled cluster reaction enthalpies involving light to heavy alkali and alkaline earth metals: the importance of sub-valence correlation. Physical Chemistry Chemical Physics, 2017, 19, 9374-9391.	2.8	43
15	Quantitative prediction of gas-phase N15 and P31 nuclear magnetic shielding constants. Journal of Chemical Physics, 2010, 132, 064109.	3.0	37
16	Interaction of Platinum Nanoparticles with Graphitic Carbon Structures: A Computational Study. ChemPhysChem, 2013, 14, 2984-2989.	2.1	36
17	DLPNO-MP2 second derivatives for the computation of polarizabilities and NMR shieldings. Journal of Chemical Physics, 2021, 154, 164110.	3.0	35
18	Full configuration-interaction and coupled-cluster calculations of the indirect spinâ€“spin coupling constant of BH. Chemical Physics Letters, 2003, 368, 172-176.	2.6	32

#	Article	IF	Citations
19	Quantitative prediction of gas-phase O17 nuclear magnetic shielding constants. Journal of Chemical Physics, 2009, 131, 024116.	3.0	31
20	Modelling electrified interfaces in quantum chemistry: constant charge vs. constant potential. Physical Chemistry Chemical Physics, 2013, 15, 2712.	2.8	31
21	Theoretical Study of Twin Polymerization â€“ From Chemical Reactivity to Structure Formation. Macromolecular Theory and Simulations, 2012, 21, 615-628.	1.4	30
22	Thermally Induced Twin Polymerization of 4Hâ€1,3,2â€Benzodioxasilines. Chemistry - A European Journal, 2014, 20, 8040-8053.	3.3	30
23	High-level ab-initio calculation of gas-phase NMR chemical shifts and secondary isotope effects of methanol. Chemical Physics Letters, 2009, 467, 230-232.	2.6	29
24	The first microsolvation step for furans: New experiments and benchmarking strategies. Journal of Chemical Physics, 2020, 152, 164303.	3.0	28
25	Microporous Carbon and Mesoporous Silica by Use of Twin Polymerization: An Integrated Experimental and Theoretical Approach to Precursor Reactivity. ChemPlusChem, 2014, 79, 1009-1023.	2.8	27
26	A Supported Bismuth Halide Perovskite Photocatalyst for Selective Aliphatic and Aromatic Câ€“H Bond Activation. Angewandte Chemie, 2020, 132, 5837-5845.	2.0	27
27	Evaluation of dispersion type metalÂ·Â·Â·Ï€ arene interaction in arylbismuth compounds â€“ an experimental and theoretical study. Beilstein Journal of Organic Chemistry, 2018, 14, 2125-2145.	2.2	25
28	Highâ€Level Ab Initio Calculations of Intermolecular Interactions: Heavy Mainâ€Group Element Ï€â€Interactions. Chemistry - A European Journal, 2018, 24, 10238-10245.	3.3	22
29	Porous Ge@C materials via twin polymerization of germanium(<scp>ii</scp>) salicyl alcoholates for Li-ion batteries. Journal of Materials Chemistry A, 2016, 4, 2705-2719.	10.3	21
30	Computation of NMR Shielding Constants for Solids Using an Embedded Cluster Approach with DFT, Double-Hybrid DFT, and MP2. Journal of Chemical Theory and Computation, 2020, 16, 6950-6967.	5.3	21
31	Constant chemical potential approach for quantum chemical calculations in electrocatalysis. Beilstein Journal of Nanotechnology, 2014, 5, 668-676.	2.8	17
32	Triple Resonance Experiments for the Rapid Detection of ¹⁰³Rh NMR Shifts: A Combined Experimental and Theoretical Study into Dirhodium and Bismuthâ€“Rhodium Paddlewheel Complexes. Journal of the American Chemical Society, 2021, 143, 12473-12479.	13.7	16
33	Structure and Reactivity of IrO_x Nanoparticles for the Oxygen Evolution Reaction in Electrocatalysis: An Electronic Structure Theory Study. Journal of Physical Chemistry C, 2021, 125, 4379-4390.	3.1	15
34	High resolution transmission electron microscopy and electronic structure theory investigation of platinum nanoparticles on carbon black. Journal of Chemical Physics, 2019, 150, 041705.	3.0	14
35	Structure and Reactivity of 1,8-Bis(naphthalenediyl)dipnictanes. Organometallics, 2019, 38, 2927-2942.	2.3	11
36	Balancing Donorâ€Acceptor and Dispersion Effects in Heavy Main Group Element Ï€ Interactions: Effect of Substituents on the Pnictogenâ‹…â‹…â‹…Ï€ Arene Interaction. ChemPhysChem, 2019, 20, 2539-2552.	2.1	10

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37	A case study of density functional theory and domain-based local pair natural orbital coupled cluster for vibrational effects on EPR hyperfine coupling constants: vibrational perturbation theory versus ab initio molecular dynamics. Molecular Physics, 2020, 118, e1797916.	1.7	9
38	Studying Natural Buckyballs and Buckybowls in Fossil Materials. Angewandte Chemie - International Edition, 2020, 59, 15008-15013.	13.8	8
39	Investigating the stability of graphitic carbon materials in electrocatalysis using electronic structure methods. Carbon, 2021, 171, 618-633.	10.3	7
40	Evaluation of bismuth-based dispersion energy donors â€“ synthesis, structure and theoretical study of 2-biphenylbismuth(<scp>iii</scp>) derivatives. Physical Chemistry Chemical Physics, 2020, 22, 10189-10211.	2.8	5
41	Are Heavy Pnictogenâ€Ï€ Interactions Really â€œÏ€ Interactionsâ€?. Chemistry - A European Journal, 2021, 27, 14520-14526.	3.3	5
42	Identifying Stereoisomers by ab-initio Calculation of Secondary Isotope Shifts on NMR Chemical Shieldings. Molecules, 2014, 19, 5301-5312.	3.8	4
43	Electronic Structure Calculations and Experimental Studies on the Thermal Initiation of the Twin Polymerization Process. ChemPlusChem, 2017, 82, 1396-1407.	2.8	4
44	High Level Electronic Structure Calculation of Molecular Solid-State NMR Shielding Constants. Journal of Chemical Theory and Computation, 2022, 18, 2408-2417.	5.3	4
45	MAXNET Energy â€“ Focusing Research in Chemical Energy Conversion on the Electrocatlytic Oxygen Evolution. Green, 2015, 5, .	0.4	3
46	Comparing London dispersion pnictogenâ€“Ï€ interactions in naphthyl-substituted dipnictanes. Dalton Transactions, 2022, 51, 5016-5023.	3.3	2
47	Studying Natural Buckyballs and Buckybowls in Fossil Materials. Angewandte Chemie, 2020, 132, 15118-15123.	2.0	1
48	An introduction to electrochemical energy conversion. EPJ Web of Conferences, 2020, 246, 00018.	0.3	0