Andreas W GÃ¶tz

List of Publications by Year
in descending order

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72 papers	8,026 citations	201674 27 h-index	91884 69 g-index
91 all docs	91 docs citations	91 times ranked	9314 citing authors

#	Article	IF	Citations
1	MÃ¶ssbauer Property Calculations on Fea33+â^™â^™â^™H2Oâ^™â^™â^™CuB2+ Dinuclear Center Models of the Resting Oxidized asâ€Isolated Cytochrome c Oxidase. ChemPhysChem, 2022, , .	2.1	2
2	Uptake of N2O5 by aqueous aerosol unveiled using chemically accurate many-body potentials. Nature Communications, 2022, 13, 1266.	12.8	8
3	Computer-aided drug design, quantum-mechanical methods for biological problems. Current Opinion in Structural Biology, 2022, 75, 102417.	5.7	10
4	Structure, Electronic, and Charge Transfer Properties of Organic Photovoltaics from Density Functional Theory Methods. Challenges and Advances in Computational Chemistry and Physics, 2021, , 57-79.	0.6	0
5	Open-Source Multi-GPU-Accelerated QM/MM Simulations with AMBER and QUICK. Journal of Chemical Information and Modeling, 2021, 61, 2109-2115.	5.4	19
6	Highly Accurate Many-Body Potentials for Simulations of N₂O₅ in Water: Benchmarks, Development, and Validation. Journal of Chemical Theory and Computation, 2021, 17, 3931-3945.	5.3	13
7	Harnessing the Power of Multi-GPU Acceleration into the Quantum Interaction Computational Kernel Program. Journal of Chemical Theory and Computation, 2021, 17, 3955-3966.	5.3	15
8	MB-Fit: Software infrastructure for data-driven many-body potential energy functions. Journal of Chemical Physics, 2021, 155, 124801.	3.0	18
9	Data for molecular dynamics simulations of Escherichia coli cytochrome bd oxidase with the Amber force field. Data in Brief, 2021, 38, 107401.	1.0	1
10	Solvation Free Energies and Adsorption Energies at the Metal/Water Interface from Hybrid Quantum-Mechanical/Molecular Mechanics Simulations. Journal of Chemical Theory and Computation, 2020, 16, 6539-6549.	5.3	34
11	Coupled transport of electrons and protons in a bacterial cytochromecoxidaseâ€”DFT calculated properties compared to structures and spectroscopies. Physical Chemistry Chemical Physics, 2020, 22, 26652-26668.	2.8	12
12	ReaxFF/AMBERâ€”A Framework for Hybrid Reactive/Nonreactive Force Field Molecular Dynamics Simulations. Journal of Chemical Theory and Computation, 2020, 16, 7645-7654.	5.3	19
13	NWChem: Past, present, and future. Journal of Chemical Physics, 2020, 152, 184102.	3.0	425
14	A Water Molecule Residing in the Fea33+Â·Â·Â·CuB2+Dinuclear Center of the Resting Oxidized as-Isolated CytochromecOxidase: A Density Functional Study. Inorganic Chemistry, 2020, 59, 8906-8915.	4.0	10
15	Parallel Implementation of Density Functional Theory Methods in the Quantum Interaction Computational Kernel Program. Journal of Chemical Theory and Computation, 2020, 16, 4315-4326.	5.3	25
16	Low-order many-body interactions determine the local structure of liquid water. Chemical Science, 2019, 10, 8211-8218.	7.4	35
17	DFT Fe_{a3}â€“O/Oâ€“O Vibrational Frequency Calculations over Catalytic Reaction Cycle States in the Dinuclear Center of Cytochrome c Oxidase. Inorganic Chemistry, 2019, 58, 13933-13944.	4.0	11
18	Van der Waals effects on structure and optical properties in organic photovoltaics. International Journal of Quantum Chemistry, 2019, 119, e25883.	2.0	8

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19	Molecular QTAIM Topology Is Sensitive to Relativistic Corrections. Chemistry - A European Journal, 2019, 25, 2538-2544.	3.3	9
20	Comparison of permutationally invariant polynomials, neural networks, and Gaussian approximation potentials in representing water interactions through many-body expansions. Journal of Chemical Physics, 2018, 148, 241725.	3.0	142
21	A Water Dimer Shift Activates a Proton Pumping Pathway in the P_R â†' F Transition of ba₃ Cytochrome c Oxidase. Inorganic Chemistry, 2018, 57, 1048-1059.	4.0	11
22	Force Field for Water over Pt(111): Development, Assessment, and Comparison. Journal of Chemical Theory and Computation, 2018, 14, 3238-3251.	5.3	38
23	N₂O₅at water surfaces: binding forces, charge separation, energy accommodation and atmospheric implications. Physical Chemistry Chemical Physics, 2018, 20, 17961-17976.	2.8	18
24	Monitoring Water Clusters â€œMeltâ€•Through Vibrational Spectroscopy. Journal of the American Chemical Society, 2017, 139, 7082-7088.	13.7	69
25	Combined quantumâ€•mechanical molecular mechanics calculations with NWChem and AMBER: Excited state properties of green fluorescent protein chromophore analogue in aqueous solution. Journal of Computational Chemistry, 2017, 38, 1631-1639.	3.3	3
26	Analytical gradients for subsystem density functional theory within the slaterâ€functionâ€based amsterdam density functional program. Journal of Computational Chemistry, 2017, 38, 238-249.	3.3	10
27	Effects of Dispersion Forces on Structure and Photoinduced Charge Separation in Organic Photovoltaics. Journal of Physical Chemistry C, 2017, 121, 20134-20140.	3.1	14
28	Molecular mechanics models for the image charge, a comment on â€œincluding image charge effects in the molecular dynamics simulations of molecules on metal surfacesâ€• Journal of Computational Chemistry, 2017, 38, 2127-2129.	3.3	9
29	Toward chemical accuracy in the description of ionâ€“water interactions through many-body representations. Alkali-water dimer potential energy surfaces. Journal of Chemical Physics, 2017, 147, 161715.	3.0	57
30	Relativistic (SRâ€ZORA) quantum theory of atoms in molecules properties. Journal of Computational Chemistry, 2017, 38, 81-86.	3.3	12
31	On the accuracy of the MB-pol many-body potential for water: Interaction energies, vibrational frequencies, and classical thermodynamic and dynamical properties from clusters to liquid water and ice. Journal of Chemical Physics, 2016, 145, 194504.	3.0	214
32	A broken-symmetry density functional study of structures, energies, and protonation states along the catalytic Oâ€“O bond cleavage pathway in ba3 cytochrome c oxidase from Thermus thermophilus. Physical Chemistry Chemical Physics, 2016, 18, 21162-21171.	2.8	21
33	Toward Chemical Accuracy in the Description of Ionâ€“Water Interactions through Many-Body Representations. I. Halideâ€“Water Dimer Potential Energy Surfaces. Journal of Chemical Theory and Computation, 2016, 12, 2698-2705.	5.3	81
34	Data for molecular dynamics simulations of B-type cytochrome c oxidase with the Amber force field. Data in Brief, 2016, 8, 1209-1214.	1.0	13
35	The i-TTM model for ab initio-based ionâ€“water interaction potentials. II. Alkali metal ionâ€“water potential energy functions. Physical Chemistry Chemical Physics, 2016, 18, 30334-30343.	2.8	43
36	Water exit pathways and proton pumping mechanism in B-type cytochrome c oxidase from molecular dynamics simulations. Biochimica Et Biophysica Acta - Bioenergetics, 2016, 1857, 1594-1606.	1.0	15

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37	A QTAIM topological analysis of the P3HTâ¿¿PCBM dimer. Chemical Physics Letters, 2016, 644, 157-162.	2.6	8
38	The adaptive buffered force <scp>QM/MM</scp> method in the <scp>CP2K</scp> and <scp>AMBER</scp> software packages. Journal of Computational Chemistry, 2015, 36, 633-648.	3.3	39
39	Electronic Structure of Ni₂E₂ Complexes (E = S, Se, Te) and a Global Analysis of M₂E₂ Compounds: A Case for Quantized E₂^{nâ€“} Oxidation Levels with n = 2, 3, or 4. Journal of the American Chemical Society, 2015, 137, 4993-5011.	13.7	26
40	On the representation of many-body interactions in water. Journal of Chemical Physics, 2015, 143, 104102.	3.0	80
41	Cisplatin inhibits MEK1/2. Oncotarget, 2015, 6, 23510-23522.	1.8	7
42	An extensible interface for QM/MM molecular dynamics simulations with AMBER. Journal of Computational Chemistry, 2014, 35, 95-108.	3.3	130
43	Calculation of nuclear spin-spin coupling constants using frozen density embedding. Journal of Chemical Physics, 2014, 140, 104107.	3.0	13
44	Linking Chemical Electronâ€“Proton Transfer to Proton Pumping in Cytochrome c Oxidase: Broken-Symmetry DFT Exploration of Intermediates along the Catalytic Reaction Pathway of the Ironâ€“Copper Dinuclear Complex. Inorganic Chemistry, 2014, 53, 6458-6472.	4.0	38
45	Structural and electronic properties of the P3HTâ€“PCBM dimer: A theoretical Study. Chemical Physics Letters, 2014, 612, 234-239.	2.6	17
46	The Mechanism of Cellulose Hydrolysis by a Two-Step, Retaining Cellobiohydrolase Elucidated by Structural and Transition Path Sampling Studies. Journal of the American Chemical Society, 2014, 136, 321-329.	13.7	164
47	Dipeptide Aggregation in Aqueous Solution from Fixed Point-Charge Force Fields. Journal of Chemical Theory and Computation, 2014, 10, 1631-1637.	5.3	10
48	Routine Microsecond Molecular Dynamics Simulations with AMBER on GPUs. 2. Explicit Solvent Particle Mesh Ewald. Journal of Chemical Theory and Computation, 2013, 9, 3878-3888.	5.3	2,598
49	SPFP: Speed without compromiseâ€”A mixed precision model for GPU accelerated molecular dynamics simulations. Computer Physics Communications, 2013, 184, 374-380.	7.5	881
50	Bond energy decomposition analysis for subsystem density functional theory. Journal of Chemical Physics, 2013, 138, 094113.	3.0	14
51	Electronic Absorption Spectra from MM and ab Initio QM/MM Molecular Dynamics: Environmental Effects on the Absorption Spectrum of Photoactive Yellow Protein. Journal of Chemical Theory and Computation, 2012, 8, 5092-5106.	5.3	158
52	Application of Adaptive QM/MM Methods to Molecular Dynamics Simulations of Aqueous Systems. Journal of Chemical Theory and Computation, 2012, 8, 2868-2877.	5.3	54
53	Routine Microsecond Molecular Dynamics Simulations with AMBER on GPUs. 1. Generalized Born. Journal of Chemical Theory and Computation, 2012, 8, 1542-1555.	5.3	1,633
54	Xâ€ray Absorption Spectroscopic, Crystallographic, Theoretical (DFT) and Chemical Evidence for a Chalcogenâ€“Chalcogen Twoâ€Center/Threeâ€Electron Half Bond in an Unprecedented â€œSubselenideâ€• Se₂^{3â^’} Ligand. Chemistry - A European Journal, 2012, 18, 9179-9183.	3.3	13

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55	Computational Study on the Anomalous Fluorescence Behavior of Isoflavones. Journal of Physical Chemistry A, 2011, 115, 1493-1499.	2.5	17
56	PyADF â€" A scripting framework for multiscale quantum chemistry. Journal of Computational Chemistry, 2011, 32, 2328-2338.	3.3	71
57	Density-Functional Theory with Orbital-Dependent Functionals: Exact-exchange Kohn-Sham and Density-Functional Response Methods. Zeitschrift Fur Physikalische Chemie, 2010, 224, 325-342.	2.8	16
58	The weak covalent bond in NgAuF (Ng=Ar, Kr, Xe): A challenge for subsystem density functional theory. Journal of Chemical Physics, 2010, 132, 044114.	3.0	41
59	Quantum Chemistry on Graphics Processing Units. Annual Reports in Computational Chemistry, 2010, , 21-35.	1.7	24
60	Virial theorem in the Kohnâ€"Sham density-functional theory formalism: Accurate calculation of the atomic quantum theory of atoms in molecules energies. Journal of Chemical Physics, 2009, 131, 021101.	3.0	48
61	A high performance grid-based algorithm for computing QTAIM properties. Chemical Physics Letters, 2009, 472, 149-152.	2.6	151
62	Performance of Kinetic Energy Functionals for Interaction Energies in a Subsystem Formulation of Density Functional Theory. Journal of Chemical Theory and Computation, 2009, 5, 3161-3174.	5.3	109
63	Suitability of III-V<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:mrow><mml:mo>[</mml:mo><mml:mrow><mml:mi>X</mml:mi><mml:msub><mml:mtext>H</m for hydrogen storage: A density functional study. Physical Review B, 2009, 79, .	3.2	0
64	Numerically stable optimized effective potential method with balanced Gaussian basis sets. Journal of Chemical Physics, 2007, 127, 054102.	3.0	130
65	Alternative Synthesis, Density Functional Calculations and Proton Reactivity Study of a Trinuclear [NiFe] Hydrogenase Model Compound. European Journal of Inorganic Chemistry, 2007, 2007, 3385-3393.	2.0	10
66	An indirect approach to the determination of the nuclear quadrupole moment by four-component relativistic DFT in molecular calculations. Chemical Physics Letters, 2007, 442, 233-237.	2.6	14
67	Hydrazine Nitrosation of a Metal-Bound Nitric Oxide:â€‰ Structural Evidence for the Formation of an Ammine Complex. Inorganic Chemistry, 2006, 45, 4661-4667.	4.0	3
68	Diastereoselective Synthesis of Arene Ruthenium(II) Complexes Containing Chiral Phosphetane-Based Tethersâ€‚1. Organometallics, 2006, 25, 2607-2616.	2.3	28
69	Optimization of auxiliary basis sets for the LEDO expansion and a projection technique for LEDO-DFT. Journal of Computational Chemistry, 2005, 26, 1242-1253.	3.3	3
70	Analytical gradients for LEDO-DFT. Molecular Physics, 2005, 103, 175-182.	1.7	3
71	A Quantum Chemical Study of Racemization Pathways in Substituted Chrysene Derivatives. Chemistry - A European Journal, 2003, 9, 1610-1619.	3.3	0
72	Phthalic acid, a versatile building block in organic-organometallic crystal engineering. New Journal of Chemistry, 1999, 23, 17-24.	2.8	20