Sebastian HÃ¶fener

List of Publications by Year
in descending order

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Version: 2024-02-01

49 papers	1,548 citations	430874 18 h-index	302126 39 g-index
49 all docs	49 docs citations	49 times ranked	1900 citing authors

#	Article	IF	Citations
1	Optimized accurate auxiliary basis sets for RI-MP2 and RI-CC2 calculations for the atoms Rb to Rn. Theoretical Chemistry Accounts, 2007, 117, 587-597.	1.4	577
2	The MP2â€F12 method in the T<scp>URBOMOLE</scp> program package. Journal of Computational Chemistry, 2011, 32, 2492-2513.	3.3	98
3	Molecular properties via a subsystem density functional theory formulation: A common framework for electronic embedding. Journal of Chemical Physics, 2012, 136, 044104.	3.0	90
4	Scope and limitations of the SCS-MP2 method for stacking and hydrogen bonding interactions. Physical Chemistry Chemical Physics, 2008, 10, 2758.	2.8	80
5	Solvatochromic shifts from coupled-cluster theory embedded in density functional theory. Journal of Chemical Physics, 2013, 139, 104106.	3.0	50
6	Fluorescence behavior of (selected) flavonols: a combined experimental and computational study. Physical Chemistry Chemical Physics, 2013, 15, 12572.	2.8	49
7	Slater-type geminals in explicitly-correlated perturbation theory: application to n-alkanols and analysis of errors and basis-set requirements. Physical Chemistry Chemical Physics, 2008, 10, 3390.	2.8	38
8	Coupledâ€cluster frozenâ€density embedding using resolution of the identity methods. Journal of Computational Chemistry, 2014, 35, 1716-1724.	3.3	38
9	Benchmark and performance of long-range corrected time-dependent density functional tight binding (LC-TD-DFTB) on rhodopsins and light-harvesting complexes. Physical Chemistry Chemical Physics, 2020, 22, 10500-10518.	2.8	36
10	Calculation of electronic excitations using wave-function in wave-function frozen-density embedding. Journal of Chemical Physics, 2012, 137, 204120.	3.0	34
11	Effects of counterpoise correction and basis set extrapolation on the MP2 geometries of hydrogen bonded dimers of ammonia, water, and hydrogen fluoride. Physical Chemistry Chemical Physics, 2011, 13, 1230-1238.	2.8	31
12	Wave Function Frozen-Density Embedding: Coupled Excitations. Journal of Chemical Theory and Computation, 2016, 12, 549-557.	5.3	29
13	Explicitly correlated second-order perturbation theory calculations on molecules containing heavy main-group elements. Theoretical Chemistry Accounts, 2008, 121, 11-19.	1.4	27
14	Natural transition orbitals for the calculation of correlation and excitation energies. Chemical Physics Letters, 2017, 679, 52-59.	2.6	25
15	The geminal basis in explicitly correlated wave functions. Chemical Physics, 2009, 356, 25-30.	1.9	24
16	Origin of the Argon Nanocoating Shift in the OH Stretching Fundamental of n-Propanol: A Combined Experimental and Quantum Chemical Study. Journal of Physical Chemistry C, 2009, 113, 10929-10938.	3.1	23
17	Computing UV/vis spectra using a combined molecular dynamics and quantum chemistry approach: bis-triazin-pyridine (BTP) ligands studied in solution. Physical Chemistry Chemical Physics, 2016, 18, 7728-7736.	2.8	21
18	Analytical nuclear gradients of the explicitly correlated MÃ¸llerâ€“Plesset second-order energy. Molecular Physics, 2010, 108, 1783-1796.	1.7	19

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19	Relativistic and Nonâ€Relativistic Electronic Molecularâ€Structure Calculations for Dimers of 4pâ€, 5pâ€, and 6pâ€Block Elements. ChemPhysChem, 2012, 13, 3952-3957.	2.1	18
20	Numerically accurate linear response-properties in the configuration-interaction singles (CIS) approximation. Physical Chemistry Chemical Physics, 2015, 17, 31453-31462.	2.8	18
21	Photophysical Properties of Benzoylgermane and paraâ€Substituted Derivatives: Substituent Effects on Electronic Transitions. ChemPhysChem, 2016, 17, 3460-3469.	2.1	17
22	Frozen-Density Embedding Potentials and Chiroptical Properties. Journal of Chemical Theory and Computation, 2015, 11, 5305-5315.	5.3	16
23	Similarities and differences of the Lagrange formalism and the intermediate state representation in the treatment of molecular properties. Journal of Chemical Physics, 2019, 150, 164125.	3.0	15
24	Waveâ€function frozenâ€density embedding: Approximate analytical nuclear groundâ€state gradients. Journal of Computational Chemistry, 2016, 37, 1092-1101.	3.3	14
25	Unexpected Trimerization of Pyrazine in the Coordination Sphere of Low-Valent Titanocene Fragments. Journal of Chemical Theory and Computation, 2009, 5, 2044-2049.	5.3	12
26	Twisting the TAPPs: Bay â€Substituted Nonâ€planar Tetraazaperoâ€pyrenes and their Reduced Anions. Chemistry - A European Journal, 2019, 25, 14669-14678.	3.3	12
27	Analytic Calculation of First-order Molecular Properties at the Explicitly-correlated Second-order MÃ¸ller-Plesset Level. Zeitschrift Fur Physikalische Chemie, 2010, 224, 695-708.	2.8	11
28	Analytical nuclear gradients for electron-attached and electron-detached states for the second-order algebraic diagrammatic construction scheme combined with frozen-density embedding. Journal of Chemical Physics, 2020, 152, 174109.	3.0	10
29	Analytical Time-Dependent Long-Range Corrected Density Functional Tight Binding (TD-LC-DFTB) Gradients in DFTB+: Implementation and Benchmark for Excited-State Geometries and Transition Energies. Journal of Chemical Theory and Computation, 2021, 17, 2266-2282.	5.3	10
30	Analytical nuclear excitedâ€state gradients for the Tammâ€“Dancoff approximation using uncoupled frozenâ€density embedding. Journal of Computational Chemistry, 2017, 38, 2316-2325.	3.3	9
31	Communication: Biological applications of coupled-cluster frozen-density embedding. Journal of Chemical Physics, 2018, 148, 141101.	3.0	9
32	Understanding UVâ€“Vis Spectra of Halogenated Tetraazaperopyrenes (TAPPs): A Computational Study. Journal of Physical Chemistry A, 2019, 123, 3160-3169.	2.5	9
33	Perhalogenated Tetraazaperopyrenes and Their Corresponding Mono- and Dianions. Organic Letters, 2020, 22, 2298-2302.	4.6	9
34	Combining frozenâ€density embedding with the conductorâ€like screening model using <scp>L</scp>agrangian techniques for response properties. Journal of Computational Chemistry, 2017, 38, 1693-1703.	3.3	8
35	The <scp>KOALA</scp> program: Wavefunction frozenâ€density embedding. International Journal of Quantum Chemistry, 2021, 121, e26351.	2.0	8
36	Ultrafast Singlet Fission and Intersystem Crossing in Halogenated Tetraazaperopyrenes. Journal of Physical Chemistry A, 2020, 124, 7857-7868.	2.5	7

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37	Employing Pseudopotentials to Tackle Excited-State Electron Spill-Out in Frozen Density Embedding Calculations. Journal of Chemical Theory and Computation, 2022, 18, 1737-1747.	5.3	7
38	Solvatochromic shifts of Br₂ and I₂ in water cages of type 5¹², 5¹²6², 5¹²6³, and 5¹²6⁴. Journal of Computational Chemistry, 2015, 36, 853-860.	3.3	6
39	Geometry dependence of excitonic couplings and the consequences for configurationâ€space sampling. Journal of Computational Chemistry, 2021, 42, 1402-1418.	3.3	5
40	Analytical Nuclear Excited-State Gradients for the Second-Order Approximate Coupled-Cluster Singles and Doubles (CC2) Method Employing Uncoupled Frozen-Density Embedding. Journal of Chemical Theory and Computation, 2018, 14, 4616-4628.	5.3	4
41	Frozen-density embedding employing configuration interaction as a subsystem method. Molecular Physics, 2020, 118, e1665726.	1.7	4
42	Combining wavefunction frozen-density embedding with one-dimensional periodicity. Journal of Chemical Physics, 2021, 154, 104114.	3.0	4
43	Calculation of the two-electron Darwin term using explicitly correlated wave functions. Chemical Physics, 2012, 401, 146-151.	1.9	3
44	The extended explicitly-correlated second-order approximate coupled-cluster singles and doubles ansatz suitable for response theory. Journal of Chemical Physics, 2019, 150, 184110.	3.0	3
45	Origin of the Solvatochromism in Organic Fluorophores with Flexible Side Chains: A Case Study of Flugi-2. Journal of Physical Chemistry A, 2019, 123, 4581-4587.	2.5	3
46	A Fock-operator complete active space self-consistent field (CAS-SCF) method combined with frozen-density embedding. Journal of Chemical Physics, 2021, 154, 084120.	3.0	3
47	The influence of polarity in binary solvent mixtures on the conformation of bis-triazinyl-pyridine in solution. Molecular Physics, 2018, 116, 507-514.	1.7	2
48	Understanding excited state properties of host materials in OLEDs: simulation of absorption spectrum of amorphous 4,4-bis(carbazol-9-yl)-2,2-biphenyl (CBP). Physical Chemistry Chemical Physics, 2022, , .	2.8	2
49	Effects of rotational conformation on electronic properties of 4,4â€²-bis(carbazol-9-yl)biphenyl (CBP): the single-molecule picture and beyond. Molecular Physics, 2021, 119, e1876936.	1.7	1