Thomas MÃ¼ller

List of Publications by Year
in descending order

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35 papers	4,616 citations	186265 28 h-index	345221 36 g-index
37 all docs	37 docs citations	37 times ranked	4644 citing authors

#	Article	IF	Citations
1	TURBOMOLE: Modular program suite for ab initio quantum-chemical and condensed-matter simulations. Journal of Chemical Physics, 2020, 152, 184107.	3.0	616
2	The generality of the GUGA MRCI approach in COLUMBUS for treating complex quantum chemistry. Journal of Chemical Physics, 2020, 152, 134110.	3.0	42
3	Local Electron Correlation Treatment in Extended Multireference Calculations: Effect of Acceptorâ€“Donor Substituents on the Biradical Character of the Polycyclic Aromatic Hydrocarbon Heptazethrene. Journal of Chemical Theory and Computation, 2017, 13, 2612-2622.	5.3	13
4	<scp>Molcas</scp> 8: New capabilities for multiconfigurational quantum chemical calculations across the periodic table. Journal of Computational Chemistry, 2016, 37, 506-541.	3.3	1,317
5	Polyradical Character of Triangular Non-KekulÃ© Structures, Zethrenes, p-Quinodimethane-Linked Bisphenalenyl, and the Clar Goblet in Comparison: An Extended Multireference Study. Journal of Physical Chemistry A, 2016, 120, 1625-1636.	2.5	91
6	Study of the Diradicaloid Character in a Prototypical Pancakeâ€Bonded Dimer: The Stacked Tetracyanoethylene (TCNE) Anion Dimer and the Neutral K₂TCNE₂ Complex. ChemPhysChem, 2014, 15, 165-176.	2.1	43
7	Perturbational treatment of spin-orbit coupling for generally applicable high-level multi-reference methods. Journal of Chemical Physics, 2014, 141, 074105.	3.0	33
8	A comparison of singlet and triplet states for one- and two-dimensional graphene nanoribbons using multireference theory. Theoretical Chemistry Accounts, 2014, 133, 1.	1.4	56
9	The Multiradical Character of Oneâ€and Twoâ€Dimensional Graphene Nanoribbons. Angewandte Chemie - International Edition, 2013, 52, 2581-2584.	13.8	197
10	Nonadiabatic Photodynamics of a Retinal Model in Polar and Nonpolar Environment. Journal of Physical Chemistry A, 2013, 117, 2790-2799.	2.5	55
11	Ultrafast non-adiabatic dynamics of ethylene including Rydberg states. Molecular Physics, 2013, 111, 2439-2450.	1.7	41
12	Multiconfiguration Self-Consistent Field and Multireference Configuration Interaction Methods and Applications. Chemical Reviews, 2012, 112, 108-181.	47.7	559
13	Strikingly Different Effects of Hydrogen Bonding on the Photodynamics of Individual Nucleobases in DNA: Comparison of Guanine and Cytosine. Journal of the American Chemical Society, 2012, 134, 13662-13669.	13.7	31
14	Columbusâ€”a program system for advanced multireference theory calculations. Wiley Interdisciplinary Reviews: Computational Molecular Science, 2011, 1, 191-199.	14.6	171
15	Toward an Improved Ground State Potential Energy Surface of Ozone. Journal of Physical Chemistry A, 2010, 114, 9927-9935.	2.5	68
16	The effect of hydration on the photo-deactivation pathways of 4-aminopyrimidine. Chemical Physics, 2010, 375, 110-117.	1.9	14
17	Does Stacking Restrain the Photodynamics of Individual Nucleobases?. Journal of the American Chemical Society, 2010, 132, 8261-8263.	13.7	67
18	Azomethane: Nonadiabatic Photodynamical Simulations in Solution. Journal of Physical Chemistry A, 2010, 114, 12585-12590.	2.5	43

#	Article	IF	Citations
19	Nonadiabatic Excited-State Dynamics with Hybrid ab Initio Quantum-Mechanical/Molecular-Mechanical Methods: Solvation of the Pentadieniminium Cation in Apolar Media. Journal of Physical Chemistry A, 2010, 114, 6757-6765.	2.5	74
20	Matrix-controlled photofragmentation of formamide: dynamics simulation in argon by nonadiabatic QM/MM method. Physical Chemistry Chemical Physics, 2010, 12, 12719.	2.8	29
21	Large-Scale Parallel Uncontracted Multireference-Averaged Quadratic Coupled Cluster: The Ground State of the Chromium Dimer Revisited. Journal of Physical Chemistry A, 2009, 113, 12729-12740.	2.5	85
22	The accuracy of molecular bond lengths computed by multireference electronic structure methods. Chemical Physics, 2008, 349, 37-57.	1.9	27
23	Solvent effects in electronically excited states using the continuum solvation model COSMO in combination with multireference configuration interaction with singles and doubles (MR-CISD). Theoretical Chemistry Accounts, 2004, 111, 78-89.	1.4	46
24	Electron correlation effects in N2and CO studied by X-ray scattering and CISD calculations. Molecular Physics, 2002, 100, 2839-2847.	1.7	2
25	High-level multireference methods in the quantum-chemistry program system COLUMBUS: Analytic MR-CISD and MR-AQCC gradients and MR-AQCC-LRT for excited states, GUGA spinâ€“orbit CI and parallel CI density. Physical Chemistry Chemical Physics, 2001, 3, 664-673.	2.8	401
26	A systematic theoretical investigation of the valence excited states of the diatomic molecules B 2 , C 2 , N 2 and O 2. Theoretical Chemistry Accounts, 2001, 105, 227-243.	1.4	110
27	Simultaneous calculation of Rydberg and valence excited states of formaldehyde. Theoretical Chemistry Accounts, 2001, 106, 369-378.	1.4	23
28	Geometry optimization of excited valence states of formaldehyde using analytical multireference configuration interaction singles and doubles and multireference averaged quadratic coupled-cluster gradients, and the conical intersection formed by the 1â€Š[sup 1]B[sub 1](Ïƒ-Ï€[sup â^—]) and 2â€Š[sup 1]A[sub 1](Ï€-Ï€[sup â^—]) states. Journal of Chemical Physics, 2001, 114, 746.	3.0	38
29	Excitation energies and transition moments by the multireference averaged quadratic coupled cluster (MR-AQCC) method. Physical Chemistry Chemical Physics, 2000, 2, 2067-2073.	2.8	68
30	The ethylene 1â€Š1B1uâ€ŠV state revisited. Journal of Chemical Physics, 1999, 110, 7176-7184.	3.0	86
31	A systematic ab initio investigation of the open and ring structures of ozone. Chemical Physics Letters, 1998, 293, 72-80.	2.6	53
32	Electron correlation effects in position and momentum space: the atoms Li through Ar. Computational and Theoretical Chemistry, 1996, 360, 55-65.	1.5	35
33	MR-SDCI study on high-energy electron and X-ray scattering cross-sections of linear molecules. Molecular Physics, 1996, 88, 1563-1574.	1.7	5
34	High-energy electron and X-ray scattering cross sections of N2. A MR-SDCI study. Chemical Physics Letters, 1995, 236, 497-502.	2.6	18
35	Accurate inelastic scattering factors for lithium to argon calculated from MR-SDCI wavefunctions. Chemical Physics, 1995, 191, 213-222.	1.9	36