

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
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37
all docs

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docs citations

37
times ranked

4644
citing authors

#	ARTICLE	IF	CITATIONS
1	<scp>Molcas</scp> 8: New capabilities for multiconfigurational quantum chemical calculations across the periodic table. <i>Journal of Computational Chemistry</i> , 2016, 37, 506-541.	3.3	1,317
2	TURBOMOLE: Modular program suite for <i>ab initio</i> quantum-chemical and condensed-matter simulations. <i>Journal of Chemical Physics</i> , 2020, 152, 184107.	3.0	616
3	Multiconfiguration Self-Consistent Field and Multireference Configuration Interaction Methods and Applications. <i>Chemical Reviews</i> , 2012, 112, 108-181.	47.7	559
4	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 spin-orbit CI and parallel CI density. <i>Physical Chemistry Chemical Physics</i> , 2001, 3, 664-673.	2.8	401
5	The Multiradical Character of One- and Two-Dimensional Graphene Nanoribbons. <i>Angewandte Chemie - International Edition</i> , 2013, 52, 2581-2584.	13.8	197
6	Columbus—a program system for advanced multireference theory calculations. <i>Wiley Interdisciplinary Reviews: Computational Molecular Science</i> , 2011, 1, 191-199.	14.6	171
7	A systematic theoretical investigation of the valence excited states of the diatomic molecules B ₂ , C ₂ , N ₂ and O ₂ . <i>Theoretical Chemistry Accounts</i> , 2001, 105, 227-243.	1.4	110
8	Polyradical Character of Triangular Non-Kekulé Structures, Zethrenes, <i>p</i> -Quinodimethane-Linked Bisphenalenyl, and the Clar Goblet in Comparison: An Extended Multireference Study. <i>Journal of Physical Chemistry A</i> , 2016, 120, 1625-1636.	2.5	91
9	The ethylene 1 ¹ B _{1u} state revisited. <i>Journal of Chemical Physics</i> , 1999, 110, 7176-7184.	3.0	86
10	Large-Scale Parallel Uncontracted Multireference-Averaged Quadratic Coupled Cluster: The Ground State of the Chromium Dimer Revisited. <i>Journal of Physical Chemistry A</i> , 2009, 113, 12729-12740.	2.5	85
11	Nonadiabatic Excited-State Dynamics with Hybrid <i>ab Initio</i> Quantum-Mechanical/Molecular-Mechanical Methods: Solvation of the Pentadieniminium Cation in Apolar Media. <i>Journal of Physical Chemistry A</i> , 2010, 114, 6757-6765.	2.5	74
12	Excitation energies and transition moments by the multireference averaged quadratic coupled cluster (MR-AQCC) method. <i>Physical Chemistry Chemical Physics</i> , 2000, 2, 2067-2073.	2.8	68
13	Toward an Improved Ground State Potential Energy Surface of Ozone. <i>Journal of Physical Chemistry A</i> , 2010, 114, 9927-9935.	2.5	68
14	Does Stacking Restrain the Photodynamics of Individual Nucleobases?. <i>Journal of the American Chemical Society</i> , 2010, 132, 8261-8263.	13.7	67
15	A comparison of singlet and triplet states for one- and two-dimensional graphene nanoribbons using multireference theory. <i>Theoretical Chemistry Accounts</i> , 2014, 133, 1.	1.4	56
16	Nonadiabatic Photodynamics of a Retinal Model in Polar and Nonpolar Environment. <i>Journal of Physical Chemistry A</i> , 2013, 117, 2790-2799.	2.5	55
17	A systematic <i>ab initio</i> investigation of the open and ring structures of ozone. <i>Chemical Physics Letters</i> , 1998, 293, 72-80.	2.6	53
18	Solvent effects in electronically excited states using the continuum solvation model COSMO in combination with multireference configuration interaction with singles and doubles (MR-CISD). <i>Theoretical Chemistry Accounts</i> , 2004, 111, 78-89.	1.4	46

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19	Azomethane: Nonadiabatic Photodynamical Simulations in Solution. <i>Journal of Physical Chemistry A</i> , 2010, 114, 12585-12590.	2.5	43
20	Study of the Diradicaloid Character in a Prototypical Pancake-Bonded Dimer: The Stacked Tetracyanoethylene (TCNE) Anion Dimer and the Neutral K_2 TCNE $_2$ Complex. <i>ChemPhysChem</i> , 2014, 15, 165-176.	2.1	43
21	The generality of the GUGA MRCI approach in COLUMBUS for treating complex quantum chemistry. <i>Journal of Chemical Physics</i> , 2020, 152, 134110.	3.0	42
22	Ultrafast non-adiabatic dynamics of ethylene including Rydberg states. <i>Molecular Physics</i> , 2013, 111, 2439-2450.	1.7	41
23	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 1^1B_1 and 2^1A_1 states. <i>Journal of Chemical Physics</i> , 2001, 114, 746.	3.0	38
24	Accurate inelastic scattering factors for lithium to argon calculated from MR-SDCI wavefunctions. <i>Chemical Physics</i> , 1995, 191, 213-222.	1.9	36
25	Electron correlation effects in position and momentum space: the atoms Li through Ar. <i>Computational and Theoretical Chemistry</i> , 1996, 360, 55-65.	1.5	35
26	Perturbational treatment of spin-orbit coupling for generally applicable high-level multi-reference methods. <i>Journal of Chemical Physics</i> , 2014, 141, 074105.	3.0	33
27	Strikingly Different Effects of Hydrogen Bonding on the Photodynamics of Individual Nucleobases in DNA: Comparison of Guanine and Cytosine. <i>Journal of the American Chemical Society</i> , 2012, 134, 13662-13669.	13.7	31
28	Matrix-controlled photofragmentation of formamide: dynamics simulation in argon by nonadiabatic QM/MM method. <i>Physical Chemistry Chemical Physics</i> , 2010, 12, 12719.	2.8	29
29	The accuracy of molecular bond lengths computed by multireference electronic structure methods. <i>Chemical Physics</i> , 2008, 349, 37-57.	1.9	27
30	Simultaneous calculation of Rydberg and valence excited states of formaldehyde. <i>Theoretical Chemistry Accounts</i> , 2001, 106, 369-378.	1.4	23
31	High-energy electron and X-ray scattering cross sections of N ₂ . A MR-SDCI study. <i>Chemical Physics Letters</i> , 1995, 236, 497-502.	2.6	18
32	The effect of hydration on the photo-deactivation pathways of 4-aminopyrimidine. <i>Chemical Physics</i> , 2010, 375, 110-117.	1.9	14
33	Local Electron Correlation Treatment in Extended Multireference Calculations: Effect of Acceptor-Donor Substituents on the Biradical Character of the Polycyclic Aromatic Hydrocarbon Heptazethrene. <i>Journal of Chemical Theory and Computation</i> , 2017, 13, 2612-2622.	5.3	13
34	MR-SDCI study on high-energy electron and X-ray scattering cross-sections of linear molecules. <i>Molecular Physics</i> , 1996, 88, 1563-1574.	1.7	5
35	Electron correlation effects in N ₂ and CO studied by X-ray scattering and CISD calculations. <i>Molecular Physics</i> , 2002, 100, 2839-2847.	1.7	2