Thomas-C Jagau

List of Publications by Year
in descending order

42 papers	4,611 citations	393982 19 h-index	276539 41 g-index
51 all docs	51 docs citations	51 times ranked	4706 citing authors

#	Article	IF	Citations
1	Theory of electronic resonances: fundamental aspects and recent advances. Chemical Communications, 2022, 58, 5205-5224.	2.2	18
2	Molecular Auger decay rates from complex-variable coupled-cluster theory. Journal of Chemical Physics, 2022, 156, 114117.	1.2	13
3	Photocatalyzed Transitionâ€Metalâ€Free Oxidative Crossâ€Coupling Reactions of Tetraorganoborates**. Chemistry - A European Journal, 2021, 27, 4322-4326.	1.7	14
4	Embedded equation-of-motion coupled-cluster theory for electronic excitation, ionisation, electron attachment, and electronic resonances. Molecular Physics, 2021, 119, .	0.8	17
5	Software for the frontiers of quantum chemistry: An overview of developments in the Q-Chem 5 package. Journal of Chemical Physics, 2021, 155, 084801.	1.2	518
6	Foreword: Prof. Gauss Festschrift. Molecular Physics, 2020, 118, e1817247.	0.8	0
7	In search of molecular ions for optical cycling: a difficult road. Physical Chemistry Chemical Physics, 2020, 22, 17075-17090.	1.3	20
8	Elektronische ResonanzzustÃnde â€“ warum die Energie komplex sein kann, Trendbericht Theoretische Chemie 2020, Teil 1. Nachrichten Aus Der Chemie, 2020, 68, 50-54.	0.0	1
9	Resolution-of-the-identity second-order MÃ¸llerâ€“Plesset perturbation theory with complex basis functions: Benchmark calculations and applications to strong-field ionization of polyacenes. Journal of Chemical Physics, 2020, 152, 174103.	1.2	12
10	Coupled-cluster techniques for computational chemistry: The <scp>CFOUR</scp> program package. Journal of Chemical Physics, 2020, 152, 214108.	1.2	375
11	Electroâ€Olefinationâ€”A Catalyst Free Stereoconvergent Strategy for the Functionalization of Alkenes. Chemistry - A European Journal, 2020, 26, 8382-8387.	1.7	17
12	Electrochemical Synthesis of Biaryls via Oxidative Intramolecular Coupling of Tetra(hetero)arylborates. Journal of the American Chemical Society, 2020, 142, 4341-4348.	6.6	39
13	The quest to uncover the nature of benzonitrile anion. Physical Chemistry Chemical Physics, 2020, 22, 5002-5010.	1.3	14
14	Resolution-of-the-identity approximation for complex-scaled basis functions. Journal of Chemical Physics, 2019, 151, 111101.	1.2	12
15	EOM-CC guide to Fock-space travel: the C₂ edition. Faraday Discussions, 2019, 217, 514-532.	1.6	15
16	Spectroscopy of temporary anion states: Rennerâ€“Teller coupling and electronic autodetachment in copper difluoride anion. Faraday Discussions, 2019, 217, 533-546.	1.6	13
17	A Schwarz inequality for complex basis function methods in non-Hermitian quantum chemistry. Journal of Chemical Physics, 2019, 151, 184104.	1.2	6
18	11. Watocâ€Kongress â€“ Ã¼ber 1500 theoretische Chemiker trafen sich in MÃ¼nchen. Nachrichten Aus Der Chemie, 2018, 66, 67-67.	0.0	0

#	Article	IF	Citations
19	Non-iterative triple excitations in equation-of-motion coupled-cluster theory for electron attachment with applications to bound and temporary anions. Journal of Chemical Physics, 2018, 148, 024104.	1.2	21
20	Locating Exceptional Points on Multidimensional Complex-Valued Potential Energy Surfaces. Journal of Physical Chemistry Letters, 2018, 9, 6978-6984.	2.1	26
21	Coupled-cluster treatment of molecular strong-field ionization. Journal of Chemical Physics, 2018, 148, 204102.	1.2	21
22	Understanding Processes Following Resonant Electron Attachment: Minimum-Energy Crossing Points between Anionic and Neutral Potential Energy Surfaces. Journal of Chemical Theory and Computation, 2018, 14, 4216-4223.	2.3	26
23	Characterization of the vibrational properties of copper difluoride anion and neutral ground states via direct and indirect photodetachment spectroscopy. Journal of Chemical Physics, 2018, 149, 084302.	1.2	5
24	Structure Optimization of Temporary Anions. Journal of Chemical Theory and Computation, 2018, 14, 3468-3478.	2.3	18
25	Extending Quantum Chemistry of Bound States to Electronic Resonances. Annual Review of Physical Chemistry, 2017, 68, 525-553.	4.8	136
26	Communication: Analytic gradients for the complex absorbing potential equation-of-motion coupled-cluster method. Journal of Chemical Physics, 2017, 146, 031101.	1.2	29
27	Characterizing metastable states beyond energies and lifetimes: Dyson orbitals and transition dipole moments. Journal of Chemical Physics, 2016, 144, 054113.	1.2	58
28	Investigating tunnel and above-barrier ionization using complex-scaled coupled-cluster theory. Journal of Chemical Physics, 2016, 145, 204115.	1.2	17
29	Same but Different: Dipole-Stabilized Shape Resonances in CuF^{â€“} and AgF^{â€“}. Journal of Physical Chemistry Letters, 2015, 6, 2786-2793.	2.1	55
30	Advances in molecular quantum chemistry contained in the Q-Chem 4 program package. Molecular Physics, 2015, 113, 184-215.	0.8	2,561
31	A Fresh Look at Resonances and Complex Absorbing Potentials: Density Matrix-Based Approach. Journal of Physical Chemistry Letters, 2014, 5, 310-315.	2.1	99
32	Complex Absorbing Potential Equation-of-Motion Coupled-Cluster Method Yields Smooth and Internally Consistent Potential Energy Surfaces and Lifetimes for Molecular Resonances. Journal of Physical Chemistry Letters, 2014, 5, 3078-3085.	2.1	48
33	Complex absorbing potentials within EOM-CC family of methods: Theory, implementation, and benchmarks. Journal of Chemical Physics, 2014, 141, 024102.	1.2	113
34	Stateâ€specific multireference coupledâ€cluster theory. Wiley Interdisciplinary Reviews: Computational Molecular Science, 2013, 3, 176-197.	6.2	98
35	Analytic evaluation of the dipole Hessian matrix in coupled-cluster theory. Journal of Chemical Physics, 2013, 139, 154106.	1.2	6
36	Linear-response theory for Mukherjee's multireference coupled-cluster method: Excitation energies. Journal of Chemical Physics, 2012, 137, 044116.	1.2	26

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37	Linear-response theory for Mukherjee's multireference coupled-cluster method: Static and dynamic polarizabilities. Journal of Chemical Physics, 2012, 137, 044115.	1.2	18
38	Ground and excited state geometries via Mukherjeeâ€™s multireference coupled-cluster method. Chemical Physics, 2012, 401, 73-87.	0.9	18
39	Analytic gradients for Mukherjeeâ€™s multireference coupled-cluster method using two-configurational self-consistent-field orbitals. Journal of Chemical Physics, 2010, 132, 144110.	1.2	40
40	Crystal Growth of a New Series of Complex Niobates, LnKNaNbO5 (Ln = La, Pr, Nd, Sm, Eu, Gd, and Tb): Structural Properties and Photoluminescence. Chemistry of Materials, 2009, 21, 1955-1961.	3.2	35
41	Crystal Growth, Structural Properties, and Photophysical Characterization ofLn4Na2K2M2O13(M= Nb,) Tj ETQq1 1 0.784314 rgBT /O	1.9	15
42	Computational insights into electrochemical crossâ€coupling of quaternary borate salts. Electrochemical Science Advances, 0, , e2100032.	1.2	1