

Thomas-C Jagau

List of Publications by Year in descending order

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Version: 2024-02-01

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	Advances in molecular quantum chemistry contained in the Q-Chem 4 program package. <i>Molecular Physics</i> , 2015, 113, 184-215.	0.8	2,561
2	Software for the frontiers of quantum chemistry: An overview of developments in the Q-Chem 5 package. <i>Journal of Chemical Physics</i> , 2021, 155, 084801.	1.2	518
3	Coupled-cluster techniques for computational chemistry: The <scp>CFOUR</scp> program package. <i>Journal of Chemical Physics</i> , 2020, 152, 214108.	1.2	375
4	Extending Quantum Chemistry of Bound States to Electronic Resonances. <i>Annual Review of Physical Chemistry</i> , 2017, 68, 525-553.	4.8	136
5	Complex absorbing potentials within EOM-CC family of methods: Theory, implementation, and benchmarks. <i>Journal of Chemical Physics</i> , 2014, 141, 024102.	1.2	113
6	A Fresh Look at Resonances and Complex Absorbing Potentials: Density Matrix-Based Approach. <i>Journal of Physical Chemistry Letters</i> , 2014, 5, 310-315.	2.1	99
7	State-specific multireference coupled-cluster theory. <i>Wiley Interdisciplinary Reviews: Computational Molecular Science</i> , 2013, 3, 176-197.	6.2	98
8	Characterizing metastable states beyond energies and lifetimes: Dyson orbitals and transition dipole moments. <i>Journal of Chemical Physics</i> , 2016, 144, 054113.	1.2	58
9	Same but Different: Dipole-Stabilized Shape Resonances in CuF ⁺ and AgF ⁺ . <i>Journal of Physical Chemistry Letters</i> , 2015, 6, 2786-2793.	2.1	55
10	Complex Absorbing Potential Equation-of-Motion Coupled-Cluster Method Yields Smooth and Internally Consistent Potential Energy Surfaces and Lifetimes for Molecular Resonances. <i>Journal of Physical Chemistry Letters</i> , 2014, 5, 3078-3085.	2.1	48
11	Analytic gradients for Mukherjee's multireference coupled-cluster method using two-configurational self-consistent-field orbitals. <i>Journal of Chemical Physics</i> , 2010, 132, 144110.	1.2	40
12	Electrochemical Synthesis of Biaryls via Oxidative Intramolecular Coupling of Tetra(hetero)arylborates. <i>Journal of the American Chemical Society</i> , 2020, 142, 4341-4348.	6.6	39
13	Crystal Growth of a New Series of Complex Niobates, LnKNaNbO ₅ (Ln = La, Pr, Nd, Sm, Eu, Gd, and Tb): Structural Properties and Photoluminescence. <i>Chemistry of Materials</i> , 2009, 21, 1955-1961.	3.2	35
14	Communication: Analytic gradients for the complex absorbing potential equation-of-motion coupled-cluster method. <i>Journal of Chemical Physics</i> , 2017, 146, 031101.	1.2	29
15	Linear-response theory for Mukherjee's multireference coupled-cluster method: Excitation energies. <i>Journal of Chemical Physics</i> , 2012, 137, 044116.	1.2	26
16	Locating Exceptional Points on Multidimensional Complex-Valued Potential Energy Surfaces. <i>Journal of Physical Chemistry Letters</i> , 2018, 9, 6978-6984.	2.1	26
17	Understanding Processes Following Resonant Electron Attachment: Minimum-Energy Crossing Points between Anionic and Neutral Potential Energy Surfaces. <i>Journal of Chemical Theory and Computation</i> , 2018, 14, 4216-4223.	2.3	26
18	Non-iterative triple excitations in equation-of-motion coupled-cluster theory for electron attachment with applications to bound and temporary anions. <i>Journal of Chemical Physics</i> , 2018, 148, 024104.	1.2	21

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19	Coupled-cluster treatment of molecular strong-field ionization. <i>Journal of Chemical Physics</i> , 2018, 148, 204102.	1.2	21
20	In search of molecular ions for optical cycling: a difficult road. <i>Physical Chemistry Chemical Physics</i> , 2020, 22, 17075-17090.	1.3	20
21	Linear-response theory for Mukherjee's multireference coupled-cluster method: Static and dynamic polarizabilities. <i>Journal of Chemical Physics</i> , 2012, 137, 044115.	1.2	18
22	Ground and excited state geometries via Mukherjee's multireference coupled-cluster method. <i>Chemical Physics</i> , 2012, 401, 73-87.	0.9	18
23	Structure Optimization of Temporary Anions. <i>Journal of Chemical Theory and Computation</i> , 2018, 14, 3468-3478.	2.3	18
24	Theory of electronic resonances: fundamental aspects and recent advances. <i>Chemical Communications</i> , 2022, 58, 5205-5224.	2.2	18
25	Investigating tunnel and above-barrier ionization using complex-scaled coupled-cluster theory. <i>Journal of Chemical Physics</i> , 2016, 145, 204115.	1.2	17
26	Electro-Olefination: A Catalyst Free Stereoconvergent Strategy for the Functionalization of Alkenes. <i>Chemistry - A European Journal</i> , 2020, 26, 8382-8387.	1.7	17
27	Embedded equation-of-motion coupled-cluster theory for electronic excitation, ionisation, electron attachment, and electronic resonances. <i>Molecular Physics</i> , 2021, 119, .	0.8	17
28	Crystal Growth, Structural Properties, and Photophysical Characterization of Ln ₄ Na ₂ K ₂ M ₂ O ₁₃ (M = Nb, Tj) <i>ETQq0 0,0rgBT /Oyerlock 10</i>	1.9	15
29	EOM-CC guide to Fock-space travel: the C ₂ edition. <i>Faraday Discussions</i> , 2019, 217, 514-532.	1.6	15
30	The quest to uncover the nature of benzonitrile anion. <i>Physical Chemistry Chemical Physics</i> , 2020, 22, 5002-5010.	1.3	14
31	Photocatalyzed Transition-Metal-Free Oxidative Cross-Coupling Reactions of Tetraorganoborates**. <i>Chemistry - A European Journal</i> , 2021, 27, 4322-4326.	1.7	14
32	Spectroscopy of temporary anion states: Renner-Teller coupling and electronic autodetachment in copper difluoride anion. <i>Faraday Discussions</i> , 2019, 217, 533-546.	1.6	13
33	Molecular Auger decay rates from complex-variable coupled-cluster theory. <i>Journal of Chemical Physics</i> , 2022, 156, 114117.	1.2	13
34	Resolution-of-the-identity approximation for complex-scaled basis functions. <i>Journal of Chemical Physics</i> , 2019, 151, 111101.	1.2	12
35	Resolution-of-the-identity second-order Møller-Plesset perturbation theory with complex basis functions: Benchmark calculations and applications to strong-field ionization of polyacenes. <i>Journal of Chemical Physics</i> , 2020, 152, 174103.	1.2	12
36	Analytic evaluation of the dipole Hessian matrix in coupled-cluster theory. <i>Journal of Chemical Physics</i> , 2013, 139, 154106.	1.2	6

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37	A Schwarz inequality for complex basis function methods in non-Hermitian quantum chemistry. Journal of Chemical Physics, 2019, 151, 184104.	1.2	6
38	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
39	Elektronische Resonanzzustände – warum die Energie komplex sein kann, Trendbericht Theoretische Chemie 2020, Teil 1. Nachrichten Aus Der Chemie, 2020, 68, 50-54.	0.0	1
40	Computational insights into electrochemical cross-coupling of quaternary borate salts. Electrochemical Science Advances, 0, , e2100032.	1.2	1
41	11. Watoc-Kongress – 1/4ber 1500 theoretische Chemiker trafen sich in M1/4nchen. Nachrichten Aus Der Chemie, 2018, 66, 67-67.	0.0	0
42	Foreword: Prof. Gauss Festschrift. Molecular Physics, 2020, 118, e1817247.	0.8	0