Attila Tajti

List of Publications by Year in descending order

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24 papers	1,443 citations	567281 15 h-index	610901 24 g-index
37 all docs	37 docs citations	37 times ranked	1281 citing authors

#	Article	IF	Citations
1	HEAT: High accuracy extrapolatedab initiothermochemistry. Journal of Chemical Physics, 2004, 121, 11599-11613.	3.0	691
2	Analytic calculation of the diagonal Born-Oppenheimer correction within configuration-interaction and coupled-cluster theory. Journal of Chemical Physics, 2006, 125, 144111.	3.0	182
3	Can coupled-cluster theory treat conical intersections?. Journal of Chemical Physics, 2007, 127, 044105.	3.0	81
4	Analytic evaluation of the nonadiabatic coupling vector between excited states using equation-of-motion coupled-cluster theory. Journal of Chemical Physics, 2009, 131, 124104.	3.0	56
5	Perturbative treatment of the electron-correlation contribution to the diagonal Born-Oppenheimer correction. Journal of Chemical Physics, 2007, 127, 014102.	3.0	49
6	Accuracy of Coupled Cluster Excitation Energies in Diffuse Basis Sets. Journal of Chemical Theory and Computation, 2017, 13, 202-209.	5.3	49
7	A New Benchmark Set for Excitation Energy of Charge Transfer States: Systematic Investigation of Coupled Cluster Type Methods. Journal of Chemical Theory and Computation, 2020, 16, 4213-4225.	5.3	48
8	Investigation of the Impact of Different Terms in the Second Order Hamiltonian on Excitation Energies of Valence and Rydberg States. Journal of Chemical Theory and Computation, 2016, 12, 5477-5482.	5.3	34
9	Ab initiodetermination of the heat of formation of ketenyl (HCCO) and ethynyl (CCH) radicals. Molecular Physics, 2005, 103, 2159-2168.	1.7	33
10	Reinterpretation of the UV Spectrum of Cytosine: Only Two Electronic Transitions?. ChemPhysChem, 2009, 10, 1603-1606.	2.1	29
11	Early Events in the Nonadiabatic Relaxation Dynamics of 4-(N,N-Dimethylamino)benzonitrile. Journal of Chemical Theory and Computation, 2015, 11, 1118-1128.	5.3	29
12	Accuracy of Spin-Component-Scaled CC2 Excitation Energies and Potential Energy Surfaces. Journal of Chemical Theory and Computation, 2019, 15, 5523-5531.	5.3	28
13	Accuracy of Coupled Cluster Excited State Potential Energy Surfaces. Journal of Chemical Theory and Computation, 2018, 14, 5859-5869.	5.3	24
14	Accuracy of Spin-Component Scaled ADC(2) Excitation Energies and Potential Energy Surfaces. Journal of Chemical Theory and Computation, 2020, 16, 468-474.	5.3	24
15	Code interoperability and standard data formats in quantum chemistry and quantum dynamics: The Q5/D5Cost data model. Journal of Computational Chemistry, 2014, 35, 611-621.	3.3	22
16	Diagonal Bornâ€“Oppenheimer corrections to the ground electronic state potential energy surfaces of ozone: improvement of ab initio vibrational band centers for the ¹⁶O₃, ¹⁷O₃ and ¹⁸O₃ isotopologues. Physical Chemistry Chemical Physics, 2020, 22, 24257-24269.	2.8	15
17	Improved Description of Charge-Transfer Potential Energy Surfaces via Spin-Component-Scaled CC2 and ADC(2) Methods. Journal of Chemical Theory and Computation, 2021, 17, 439-449.	5.3	14
18	Potential energy surfaces of charge transfer states. Molecular Physics, 2020, 118, e1776903.	1.7	9

#	Article	IF	Citations
19	Vibrational levels of formaldehyde: Calculations from new high precision potential energy surfaces and comparison with experimental band origins. Journal of Quantitative Spectroscopy and Radiative Transfer, 2021, 260, 107478.	2.3	9
20	Dimol Emission of Oxygen Made Possible by Repulsive Interaction. Journal of Physical Chemistry Letters, 2017, 8, 3356-3361.	4.6	5
21	On the FCNSâ‡†FC(NS) reaction: A matrix isolation and theoretical study. Journal of Molecular Spectroscopy, 2015, 310, 8-15.	1.2	4
22	Comparison of approximate intermolecular potentials for ab initio fragment calculations on medium sized Nâ€heterocycles. Journal of Computational Chemistry, 2022, 43, 1079-1093.	3.3	3
23	Efficient Sparse Matrix Algorithm to Speed Up the Calculation of the Ladder Term in Coupled Cluster Programs. Journal of Chemical Theory and Computation, 2012, 8, 3108-3118.	5.3	2
24	First-principles interpretation of electron transport through single-molecule junctions using molecular dynamics of electron attached states. Molecular Physics, 2021, 119, .	1.7	2