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	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
2	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
3	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
4	First-principles interpretation of electron transport through single-molecule junctions using molecular dynamics of electron attached states. Molecular Physics, 2021, 119, .	1.7	2
5	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
6	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
7	Potential energy surfaces of charge transfer states. Molecular Physics, 2020, 118, e1776903.	1.7	9
8	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
9	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
10	Accuracy of Coupled Cluster Excited State Potential Energy Surfaces. Journal of Chemical Theory and Computation, 2018, 14, 5859-5869.	5.3	24
11	Accuracy of Coupled Cluster Excitation Energies in Diffuse Basis Sets. Journal of Chemical Theory and Computation, 2017, 13, 202-209.	5.3	49
12	Dimol Emission of Oxygen Made Possible by Repulsive Interaction. Journal of Physical Chemistry Letters, 2017, 8, 3356-3361.	4.6	5
13	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
14	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
15	On the FCNSâ‡†FC(NS) reaction: A matrix isolation and theoretical study. Journal of Molecular Spectroscopy, 2015, 310, 8-15.	1.2	4
16	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
17	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
18	Reinterpretation of the UV Spectrum of Cytosine: Only Two Electronic Transitions?. ChemPhysChem, 2009, 10, 1603-1606.	2.1	29

#	Article	IF	Citations
19	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
20	Can coupled-cluster theory treat conical intersections?. Journal of Chemical Physics, 2007, 127, 044105.	3.0	81
21	Perturbative treatment of the electron-correlation contribution to the diagonal Born-Oppenheimer correction. Journal of Chemical Physics, 2007, 127, 014102.	3.0	49
22	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
23	Ab initiodetermination of the heat of formation of ketenyl (HCCO) and ethynyl (CCH) radicals. Molecular Physics, 2005, 103, 2159-2168.	1.7	33
24	HEAT: High accuracy extrapolatedab initiothermochemistry. Journal of Chemical Physics, 2004, 121, 11599-11613.	3.0	691