Evgeny Epifanovsky

List of Publications by Year
in descending order

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17 papers	4,097 citations	623188 14 h-index	887659 17 g-index
20 all docs	20 docs citations	20 times ranked	4573 citing authors

#	Article	IF	Citations
1	Transition states, reaction paths, and thermochemistry using the nuclearâ€“electronic orbital analytic Hessian. Journal of Chemical Physics, 2021, 154, 054108.	1.2	11
2	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
3	Coupled-Cluster Valence-Bond Singles and Doubles for Strongly Correlated Systems: Block-Tensor Based Implementation and Application to Oligoacenes. Journal of Chemical Theory and Computation, 2017, 13, 602-615.	2.3	54
4	Reducedâ€cost sparsityâ€exploiting algorithm for solving coupledâ€cluster equations. Journal of Computational Chemistry, 2016, 37, 1059-1067.	1.5	5
5	Spin-orbit couplings within the equation-of-motion coupled-cluster framework: Theory, implementation, and benchmark calculations. Journal of Chemical Physics, 2015, 143, 064102.	1.2	80
6	Advances in molecular quantum chemistry contained in the Q-Chem 4 program package. Molecular Physics, 2015, 113, 184-215.	0.8	2,561
7	Analysis and tuning of libtensor framework on multicore architectures. , 2014, , .		7
8	Investigating excited electronic states using the algebraic diagrammatic construction (ADC) approach of the polarisation propagator. Molecular Physics, 2014, 112, 774-784.	0.8	169
9	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
10	Complex absorbing potentials within EOM-CC family of methods: Theory, implementation, and benchmarks. Journal of Chemical Physics, 2014, 141, 024102.	1.2	113
11	General implementation of the resolution-of-the-identity and Cholesky representations of electron repulsion integrals within coupled-cluster and equation-of-motion methods: Theory and benchmarks. Journal of Chemical Physics, 2013, 139, 134105.	1.2	117
12	Four Bases Score a Run: Ab Initio Calculations Quantify a Cooperative Effect of H-Bonding and Ï€-Stacking on the Ionization Energy of Adenine in the AATT Tetramer. Journal of Physical Chemistry Letters, 2012, 3, 2726-2732.	2.1	43
13	Refined energetic ordering for sulphateâ€“water (nâ€‰=â€‰3â€“6) clusters using high-level electronic structure calculations. Molecular Physics, 2012, 110, 2513-2521.	0.8	22
14	Quantum Chemical Benchmark Studies of the Electronic Properties of the Green Fluorescent Protein Chromophore: 2. Cisâ^’Trans Isomerization in Water. Journal of Chemical Theory and Computation, 2009, 5, 1907-1914.	2.3	44
15	Quantum Chemical Benchmark Studies of the Electronic Properties of the Green Fluorescent Protein Chromophore. 1. Electronically Excited and Ionized States of the Anionic Chromophore in the Gas Phase. Journal of Chemical Theory and Computation, 2009, 5, 1895-1906.	2.3	109
16	On the Electronically Excited States of Uracil. Journal of Physical Chemistry A, 2008, 112, 9983-9992.	1.1	115
17	Direct location of the minimum point on intersection seams of potential energy surfaces with equation-of-motion coupled-cluster methods. Molecular Physics, 2007, 105, 2515-2525.	0.8	20