

Evgeny Epifanovsky

List of Publications by Year in descending order

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Version: 2024-02-01

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	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	Investigating excited electronic states using the algebraic diagrammatic construction (ADC) approach of the polarisation propagator. <i>Molecular Physics</i> , 2014, 112, 774-784.	0.8	169
4	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. <i>Journal of Chemical Physics</i> , 2013, 139, 134105.	1.2	117
5	On the Electronically Excited States of Uracil. <i>Journal of Physical Chemistry A</i> , 2008, 112, 9983-9992.	1.1	115
6	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
7	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. <i>Journal of Chemical Theory and Computation</i> , 2009, 5, 1895-1906.	2.3	109
8	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
9	Spin-orbit couplings within the equation-of-motion coupled-cluster framework: Theory, implementation, and benchmark calculations. <i>Journal of Chemical Physics</i> , 2015, 143, 064102.	1.2	80
10	Coupled-Cluster Valence-Bond Singles and Doubles for Strongly Correlated Systems: Block-Tensor Based Implementation and Application to Oligoacenes. <i>Journal of Chemical Theory and Computation</i> , 2017, 13, 602-615.	2.3	54
11	Quantum Chemical Benchmark Studies of the Electronic Properties of the Green Fluorescent Protein Chromophore: 2. <i>Cis</i> \rightarrow <i>Trans</i> Isomerization in Water. <i>Journal of Chemical Theory and Computation</i> , 2009, 5, 1907-1914.	2.3	44
12	Four Bases Score a Run: Ab Initio Calculations Quantify a Cooperative Effect of H-Bonding and π -Stacking on the Ionization Energy of Adenine in the AATT Tetramer. <i>Journal of Physical Chemistry Letters</i> , 2012, 3, 2726-2732.	2.1	43
13	Refined energetic ordering for sulphate-water ($n=6$) clusters using high-level electronic structure calculations. <i>Molecular Physics</i> , 2012, 110, 2513-2521.	0.8	22
14	Direct location of the minimum point on intersection seams of potential energy surfaces with equation-of-motion coupled-cluster methods. <i>Molecular Physics</i> , 2007, 105, 2515-2525.	0.8	20
15	Transition states, reaction paths, and thermochemistry using the nuclear-electronic orbital analytic Hessian. <i>Journal of Chemical Physics</i> , 2021, 154, 054108.	1.2	11
16	Analysis and tuning of libtensor framework on multicore architectures. , 2014, , .		7
17	Reduced-cost sparsity-exploiting algorithm for solving coupled-cluster equations. <i>Journal of Computational Chemistry</i> , 2016, 37, 1059-1067.	1.5	5