

Fabijan PavoÅ¾eviÄ

List of Publications by Year in descending order

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29
papers

1,420
citations

471509

17
h-index

454955

30
g-index

33
all docs

33
docs citations

33
times ranked

949
citing authors

#	ARTICLE	IF	CITATIONS
1	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.	3.0	518
2	SparseMapsâ€”A systematic infrastructure for reduced scaling electronic structure methods. V. Linear scaling explicitly correlated coupled-cluster method with pair natural orbitals. <i>Journal of Chemical Physics</i> , 2017, 146, 174108.	3.0	122
3	SparseMapsâ€”A systematic infrastructure for reduced-scaling electronic structure methods. IV. Linear-scaling second-order explicitly correlated energy with pair natural orbitals. <i>Journal of Chemical Physics</i> , 2016, 144, 144109.	3.0	98
4	Multicomponent Quantum Chemistry: Integrating Electronic and Nuclear Quantum Effects via the Nuclearâ€”Electronic Orbital Method. <i>Chemical Reviews</i> , 2020, 120, 4222-4253.	47.7	96
5	Multicomponent Coupled Cluster Singles and Doubles Theory within the Nuclear-Electronic Orbital Framework. <i>Journal of Chemical Theory and Computation</i> , 2019, 15, 338-347.	5.3	61
6	Massively Parallel Implementation of Explicitly Correlated Coupled-Cluster Singles and Doubles Using TiledArray Framework. <i>Journal of Physical Chemistry A</i> , 2016, 120, 10231-10244.	2.5	50
7	Real-Time Time-Dependent Nuclearâ€”Electronic Orbital Approach: Dynamics beyond the Bornâ€”Oppenheimer Approximation. <i>Journal of Physical Chemistry Letters</i> , 2020, 11, 4052-4058.	4.6	48
8	Development of nuclear basis sets for multicomponent quantum chemistry methods. <i>Journal of Chemical Physics</i> , 2020, 152, 244123.	3.0	47
9	Polaritonic Unitary Coupled Cluster for Quantum Computations. <i>Journal of Physical Chemistry Letters</i> , 2021, 12, 9100-9107.	4.6	33
10	Cavity-Modulated Proton Transfer Reactions. <i>Journal of the American Chemical Society</i> , 2022, 144, 4995-5002.	13.7	32
11	Multicomponent Orbital-Optimized Perturbation Theory Methods: Approaching Coupled Cluster Accuracy at Lower Cost. <i>Journal of Physical Chemistry Letters</i> , 2020, 11, 1578-1583.	4.6	31
12	Excited State Intramolecular Proton Transfer with Nuclear-Electronic Orbital Ehrenfest Dynamics. <i>Journal of Physical Chemistry Letters</i> , 2021, 12, 3497-3502.	4.6	31
13	Multicomponent equation-of-motion coupled cluster singles and doubles: Theory and calculation of excitation energies for positronium hydride. <i>Journal of Chemical Physics</i> , 2019, 150, 161102.	3.0	30
14	Enhancing the applicability of multicomponent time-dependent density functional theory. <i>Journal of Chemical Physics</i> , 2019, 150, 201101.	3.0	29
15	Multicomponent Unitary Coupled Cluster and Equation-of-Motion for Quantum Computation. <i>Journal of Chemical Theory and Computation</i> , 2021, 17, 3252-3258.	5.3	24
16	Multicomponent coupled cluster singles and doubles and Brueckner doubles methods: Proton densities and energies. <i>Journal of Chemical Physics</i> , 2019, 151, 074104.	3.0	22
17	Molecular Vibrational Frequencies within the Nuclearâ€”Electronic Orbital Framework. <i>Journal of Physical Chemistry Letters</i> , 2019, 10, 1167-1172.	4.6	22
18	Wavefunction embedding for molecular polaritons. <i>Journal of Chemical Physics</i> , 2022, 157, .	3.0	18

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19	Multicomponent Coupled Cluster Singles and Doubles with Density Fitting: Protonated Water Tetramers with Quantized Protons. <i>Journal of Physical Chemistry Letters</i> , 2021, 12, 1631-1637.	4.6	16
20	Frequency and Time Domain Nuclearâ€“Electronic Orbital Equation-of-Motion Coupled Cluster Methods: Combination Bands and Electronicâ€“Protonic Double Excitations. <i>Journal of Physical Chemistry Letters</i> , 2020, 11, 6435-6442.	4.6	15
21	Communication: Explicitly correlated formalism for second-order single-particle Greenâ€™s function. <i>Journal of Chemical Physics</i> , 2017, 147, 121101.	3.0	13
22	Thermal reaction of [3,4]-benzo-8-substituted-3Z,5Z,7E-octatetraenes and quantum-chemical study of the (8Î€,6Î€)-electrocyclisation. <i>Organic and Biomolecular Chemistry</i> , 2011, 9, 6771.	2.8	11
23	Transition states, reaction paths, and thermochemistry using the nuclearâ€“electronic orbital analytic Hessian. <i>Journal of Chemical Physics</i> , 2021, 154, 054108.	3.0	11
24	Molecular Vibrational Frequencies with Multiple Quantum Protons within the Nuclear-Electronic Orbital Framework. <i>Journal of Chemical Theory and Computation</i> , 2019, 15, 6840-6849.	5.3	10
25	Photoinduced Rearrangement of Aromatic <i>N</i> -Chloroamides to Chloroaromatic Amides in the Solid State: Inverted \hat{I}_{N} Occupational Stability of Amidyl Radicals. <i>Journal of Physical Chemistry A</i> , 2011, 115, 7834-7848.	2.5	8
26	Analytical Gradients for Nuclearâ€“Electronic Orbital Time-Dependent Density Functional Theory: Excited-State Geometry Optimizations and Adiabatic Excitation Energies. <i>Journal of Chemical Theory and Computation</i> , 2021, 17, 5110-5122.	5.3	8
27	Explicitly correlated renormalized second-order Greenâ€™s function for accurate ionization potentials of closed-shell molecules. <i>Journal of Chemical Physics</i> , 2019, 150, 214103.	3.0	6
28	Diagonal Bornâ€“Oppenheimer Corrections within the Nuclearâ€“Electronic Orbital Framework. <i>Journal of Physical Chemistry Letters</i> , 2019, 10, 4639-4643.	4.6	6
29	Multicomponent Orbital-Optimized Perturbation Theory with Density Fitting: Anharmonic Zero-Point Energies in Protonated Water Clusters. <i>Journal of Physical Chemistry Letters</i> , 2022, 13, 5563-5570.	4.6	3