Fabijan PavoÅ¡eviÄ

List of Publications by Year
in descending order

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	Cavity-Modulated Proton Transfer Reactions. Journal of the American Chemical Society, 2022, 144, 4995-5002.	13.7	32
2	Multicomponent Orbital-Optimized Perturbation Theory with Density Fitting: Anharmonic Zero-Point Energies in Protonated Water Clusters. Journal of Physical Chemistry Letters, 2022, 13, 5563-5570.	4.6	3
3	Wavefunction embedding for molecular polaritons. Journal of Chemical Physics, 2022, 157, .	3.0	18
4	Multicomponent Coupled Cluster Singles and Doubles with Density Fitting: Protonated Water Tetramers with Quantized Protons. Journal of Physical Chemistry Letters, 2021, 12, 1631-1637.	4.6	16
5	Transition states, reaction paths, and thermochemistry using the nuclearâ€“electronic orbital analytic Hessian. Journal of Chemical Physics, 2021, 154, 054108.	3.0	11
6	Excited State Intramolecular Proton Transfer with Nuclear-Electronic Orbital Ehrenfest Dynamics. Journal of Physical Chemistry Letters, 2021, 12, 3497-3502.	4.6	31
7	Multicomponent Unitary Coupled Cluster and Equation-of-Motion for Quantum Computation. Journal of Chemical Theory and Computation, 2021, 17, 3252-3258.	5.3	24
8	Analytical Gradients for Nuclearâ€“Electronic Orbital Time-Dependent Density Functional Theory: Excited-State Geometry Optimizations and Adiabatic Excitation Energies. Journal of Chemical Theory and Computation, 2021, 17, 5110-5122.	5.3	8
9	Software for the frontiers of quantum chemistry: An overview of developments in the Q-Chem 5 package. Journal of Chemical Physics, 2021, 155, 084801.	3.0	518
10	Polaritonic Unitary Coupled Cluster for Quantum Computations. Journal of Physical Chemistry Letters, 2021, 12, 9100-9107.	4.6	33
11	Frequency and Time Domain Nuclearâ€“Electronic Orbital Equation-of-Motion Coupled Cluster Methods: Combination Bands and Electronicâ€“Protonic Double Excitations. Journal of Physical Chemistry Letters, 2020, 11, 6435-6442.	4.6	15
12	Development of nuclear basis sets for multicomponent quantum chemistry methods. Journal of Chemical Physics, 2020, 152, 244123.	3.0	47
13	Multicomponent Orbital-Optimized Perturbation Theory Methods: Approaching Coupled Cluster Accuracy at Lower Cost. Journal of Physical Chemistry Letters, 2020, 11, 1578-1583.	4.6	31
14	Multicomponent Quantum Chemistry: Integrating Electronic and Nuclear Quantum Effects via the Nuclearâ€“Electronic Orbital Method. Chemical Reviews, 2020, 120, 4222-4253.	47.7	96
15	Real-Time Time-Dependent Nuclearâ˜Electronic Orbital Approach: Dynamics beyond the Bornâ€“Oppenheimer Approximation. Journal of Physical Chemistry Letters, 2020, 11, 4052-4058.	4.6	48
16	Multicomponent coupled cluster singles and doubles and Brueckner doubles methods: Proton densities and energies. Journal of Chemical Physics, 2019, 151, 074104.	3.0	22
17	Explicitly correlated renormalized second-order Greenâ€™s function for accurate ionization potentials of closed-shell molecules. Journal of Chemical Physics, 2019, 150, 214103.	3.0	6
18	Diagonal Bornâ€“Oppenheimer Corrections within the Nuclearâ€“Electronic Orbital Framework. Journal of Physical Chemistry Letters, 2019, 10, 4639-4643.	4.6	6

#	Article	IF	Citations
19	Molecular Vibrational Frequencies with Multiple Quantum Protons within the Nuclear-Electronic Orbital Framework. Journal of Chemical Theory and Computation, 2019, 15, 6840-6849.	5.3	10
20	Enhancing the applicability of multicomponent time-dependent density functional theory. Journal of Chemical Physics, 2019, 150, 201101.	3.0	29
21	Multicomponent equation-of-motion coupled cluster singles and doubles: Theory and calculation of excitation energies for positronium hydride. Journal of Chemical Physics, 2019, 150, 161102.	3.0	30
22	Molecular Vibrational Frequencies within the Nuclearâ€“Electronic Orbital Framework. Journal of Physical Chemistry Letters, 2019, 10, 1167-1172.	4.6	22
23	Multicomponent Coupled Cluster Singles and Doubles Theory within the Nuclear-Electronic Orbital Framework. Journal of Chemical Theory and Computation, 2019, 15, 338-347.	5.3	61
24	SparseMapsâ€”A systematic infrastructure for reduced scaling electronic structure methods. V. Linear scaling explicitly correlated coupled-cluster method with pair natural orbitals. Journal of Chemical Physics, 2017, 146, 174108.	3.0	122
25	Communication: Explicitly correlated formalism for second-order single-particle Greenâ€™s function. Journal of Chemical Physics, 2017, 147, 121101.	3.0	13
26	SparseMapsâ€”A systematic infrastructure for reduced-scaling electronic structure methods. IV. Linear-scaling second-order explicitly correlated energy with pair natural orbitals. Journal of Chemical Physics, 2016, 144, 144109.	3.0	98
27	Massively Parallel Implementation of Explicitly Correlated Coupled-Cluster Singles and Doubles Using TiledArray Framework. Journal of Physical Chemistry A, 2016, 120, 10231-10244.	2.5	50
28	Thermal reaction of [3,4]-benzo-8-substituted-3Z,5Z,7E-octatetraenes and quantum-chemical study of the (8Ï€,6Ï€)-electrocyclisation. Organic and Biomolecular Chemistry, 2011, 9, 6771.	2.8	11
29	Photoinduced Rearrangement of Aromatic N-Chloroamides to Chloroaromatic Amides in the Solid State: Inverted Î_Nâ€“Î£_N Occupational Stability of Amidyl Radicals. Journal of Physical Chemistry A, 2011, 115, 7834-7848.	2.5	8