Federico Zahariev

List of Publications by Year
in descending order

32 papers	1,903 citations	430874 18 h-index	454955 30 g-index
32 all docs	32 docs citations	32 times ranked	2536 citing authors

#	Article	IF	Citations
1	Recent developments in the general atomic and molecular electronic structure system. Journal of Chemical Physics, 2020, 152, 154102.	3.0	734
2	Benchmarking the performance of time-dependent density functional methods. Journal of Chemical Physics, 2012, 136, 104101.	3.0	295
3	Modeling Solvent Effects on Electronic Excited States. Journal of Physical Chemistry Letters, 2011, 2, 2184-2192.	4.6	107
4	A Paradigm for Blue- or Red-Shifted Absorption of Small Molecules Depending on the Site of Ï€-Extension. Journal of the American Chemical Society, 2010, 132, 16247-16255.	13.7	96
5	Solvent effects on optical properties of molecules: A combined time-dependent density functional theory/effective fragment potential approach. Journal of Chemical Physics, 2008, 129, 144112.	3.0	91
6	Dynamics Simulations with Spin-Flip Time-Dependent Density Functional Theory: Photoisomerization and Photocyclization Mechanisms of cis-Stilbene in Ï€Ï€* States. Journal of Physical Chemistry A, 2014, 118, 11987-11998.	2.5	84
7	Systematic Method to New Phases of Polymeric Nitrogen under High Pressure. Physical Review Letters, 2006, 97, 155503.	7.8	59
8	Solvent-Induced Shift of the Lowest Singlet Ï€ â†' Ï€* Charge-Transfer Excited State ofp-Nitroaniline in Water: An Application of the TDDFT/EFP1 Method. Journal of Physical Chemistry A, 2011, 115, 9801-9809.	2.5	49
9	Ground-State Energy as a Simple Sum of Orbital Energies in Kohn-Sham Theory: A Shift in Perspective through a Shift in Potential. Physical Review Letters, 2014, 113, 113002.	7.8	39
10	Implementation of the analytic energy gradient for the combined time-dependent density functional theory/effective fragment potential method: Application to excited-state molecular dynamics simulations. Journal of Chemical Physics, 2011, 134, 054111.	3.0	36
11	Elucidating the Nature of theStreptomyces plicatusÎ²-Hexosaminidase-Bound Intermediate Using ab initio Molecular Dynamics Simulations. Journal of the American Chemical Society, 2008, 130, 17620-17628.	13.7	35
12	Analytic Gradient for Density Functional Theory Based on the Fragment Molecular Orbital Method. Journal of Chemical Theory and Computation, 2014, 10, 5297-5307.	5.3	32
13	Functional derivatives of meta-generalized gradient approximation (meta-GGA) type exchange-correlation density functionals. Journal of Chemical Physics, 2013, 138, 244108.	3.0	31
14	Nonlinear response time-dependent density functional theory combined with the effective fragment potential method. Journal of Chemical Physics, 2014, 140, 18A523.	3.0	31
15	Combined Fragment Molecular Orbital Cluster in Molecule Approach to Massively Parallel Electron Correlation Calculations for Large Systems.. Journal of Physical Chemistry A, 2015, 119, 3587-3593.	2.5	26
16	The R^{â€“7} Dispersion Interaction in the General Effective Fragment Potential Method. Journal of Chemical Theory and Computation, 2014, 10, 1576-1587.	5.3	25
17	ParFit: A Python-Based Object-Oriented Program for Fitting Molecular Mechanics Parameters to ab Initio Data. Journal of Chemical Information and Modeling, 2017, 57, 391-396.	5.4	21
18	Silanol-Assisted Carbinolamine Formation in an Amine-Functionalized Mesoporous Silica Surface: Theoretical Investigation by Fragmentation Methods. Journal of Physical Chemistry B, 2016, 120, 1660-1669.	2.6	20

#	Article	IF	Citations
19	Predictive Beyond-Mean-Field Rate Equations for Multisite Latticeâ€“Gas Models of Catalytic Surface Reactions: CO Oxidation on Pd(100). Journal of Physical Chemistry C, 2016, 120, 28639-28653.	3.1	17
20	Ultra-fast electron capture by electrosterically-stabilized gold nanoparticles. Nanoscale, 2015, 7, 11545-11551.	5.6	16
21	Conformations of Organophosphine Oxides. Journal of Physical Chemistry A, 2015, 119, 8765-8773.	2.5	16
22	Analytic second derivative of the energy for density functional theory based on the three-body fragment molecular orbital method. Journal of Chemical Physics, 2015, 142, 124101.	3.0	12
23	Nodal variational principle for excited states. Physical Review A, 2018, 98, .	2.5	8
24	On augmented Kohnâ€“Sham potential for energy as a simple sum of orbital energies. Molecular Physics, 2016, 114, 1162-1164.	1.7	6
25	Development of a combined quantum monte carlo-effective fragment molecular orbital method. Molecular Physics, 2019, 117, 1532-1540.	1.7	4
26	Strutinsky's shell-correction method in the extended Kohn-Sham scheme for the investigation of binding energies of atoms and cations in the ground state. International Journal of Quantum Chemistry, 2004, 99, 265-276.	2.0	3
27	Properties of Augmented Kohnâ€“Sham Potential for Energy as Simple Sum of Orbital Energies. Journal of Physical Chemistry A, 2017, 121, 342-347.	2.5	3
28	Density- and spin-density-functional theories through spin-free wave functions. Physical Review A, 2019, 100, .	2.5	3
29	Combined quantum Monte Carlo â€“ effective fragment molecular orbital method: fragmentation across covalent bonds. Physical Chemistry Chemical Physics, 2021, 23, 14308-14314.	2.8	2
30	Introducing LibXC into GAMESS (US). Mendeleev Communications, 2021, 31, 302-305.	1.6	2
31	Introducing LibXC into GAMESS (US). Mendeleev Communications, 2021, 31, 302-305.	1.6	0
32	Energy components in spin-density functional theory. Physical Review A, 2021, 104, .	2.5	0