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	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
2	Introducing LibXC into GAMESS (US). Mendeleev Communications, 2021, 31, 302-305.	1.6	2
3	Introducing LibXC into GAMESS (US). Mendeleev Communications, 2021, 31, 302-305.	1.6	0
4	Energy components in spin-density functional theory. Physical Review A, 2021, 104, .	2.5	0
5	Recent developments in the general atomic and molecular electronic structure system. Journal of Chemical Physics, 2020, 152, 154102.	3.0	734
6	Development of a combined quantum monte carlo-effective fragment molecular orbital method. Molecular Physics, 2019, 117, 1532-1540.	1.7	4
7	Density- and spin-density-functional theories through spin-free wave functions. Physical Review A, 2019, 100, .	2.5	3
8	Nodal variational principle for excited states. Physical Review A, 2018, 98, .	2.5	8
9	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
10	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
11	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
12	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
13	On augmented Kohnâ€“Sham potential for energy as a simple sum of orbital energies. Molecular Physics, 2016, 114, 1162-1164.	1.7	6
14	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
15	Ultra-fast electron capture by electrosterically-stabilized gold nanoparticles. Nanoscale, 2015, 7, 11545-11551.	5.6	16
16	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
17	Conformations of Organophosphine Oxides. Journal of Physical Chemistry A, 2015, 119, 8765-8773.	2.5	16
18	Nonlinear response time-dependent density functional theory combined with the effective fragment potential method. Journal of Chemical Physics, 2014, 140, 18A523.	3.0	31

#	Article	IF	Citations
19	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
20	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
21	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
22	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
23	Functional derivatives of meta-generalized gradient approximation (meta-GGA) type exchange-correlation density functionals. Journal of Chemical Physics, 2013, 138, 244108.	3.0	31
24	Benchmarking the performance of time-dependent density functional methods. Journal of Chemical Physics, 2012, 136, 104101.	3.0	295
25	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
26	Modeling Solvent Effects on Electronic Excited States. Journal of Physical Chemistry Letters, 2011, 2, 2184-2192.	4.6	107
27	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
28	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
29	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
30	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
31	Systematic Method to New Phases of Polymeric Nitrogen under High Pressure. Physical Review Letters, 2006, 97, 155503.	7.8	59
32	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