Ksenia B Bravaya

List of Publications by Year
in descending order

Source: https://exaly.com/author-pdf/4805462/publications.pdf

Version: 2024-02-01

43	5,082	201674	243625
papers	citations	27 h-index	44 g-index

51	51	51	5458
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	Projected CAP-EOM-CCSD method for electronic resonances. Journal of Chemical Physics, 2022, 156, 094108.	3.0	9
2	The redox potential of a heme cofactor in Nitrosomonas europaea cytochrome c peroxidase: a polarizable QM/MM study. Physical Chemistry Chemical Physics, 2021, 23, 16506-16515.	2.8	8
3	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
4	Electron-induced vibrational excitation and dissociative electron attachment in methyl formate. Physical Chemistry Chemical Physics, 2020, 22, 518-524.	2.8	9
5	Effective Fragment Potentials for Flexible Molecules: Transferability of Parameters and Amino Acid Database. Journal of Chemical Theory and Computation, 2020, 16, 7735-7747.	5.3	11
6	eMap: A Web Application for Identifying and Visualizing Electron or Hole Hopping Pathways in Proteins. Journal of Physical Chemistry B, 2019, 123, 6946-6951.	2.6	16
7	Polarizable embedding for simulating redox potentials of biomolecules. Physical Chemistry Chemical Physics, 2019, 21, 11642-11650.	2.8	20
8	Dipole-Supported Electronic Resonances Mediate Electron-Induced Amide Bond Cleavage. Physical Review Letters, 2019, 122, 073002.	7.8	17
9	CAP-XMCQDPT2 method for molecular electronic resonances. Journal of Chemical Physics, 2017, 146, .	3.0	28
10	Extending Quantum Chemistry of Bound States to Electronic Resonances. Annual Review of Physical Chemistry, 2017, 68, 525-553.	10.8	136
11	First-Principles Models for Biological Light-Harvesting: Phycobiliprotein Complexes from Cryptophyte Algae. Journal of the American Chemical Society, 2017, 139, 7803-7814.	13.7	41
12	Photoinduced Chemistry in Fluorescent Proteins: Curse or Blessing?. Chemical Reviews, 2017, 117, 758-795.	47.7	203
13	Free Energies of Redox Half-Reactions from First-Principles Calculations. Journal of Physical Chemistry Letters, 2016, 7, 2490-2495.	4.6	28
14	Turning On and Off Photoinduced Electron Transfer in Fluorescent Proteins by Ï€-Stacking, Halide Binding, and Tyr145 Mutations. Journal of the American Chemical Society, 2016, 138, 4807-4817.	13.7	52
15	Electronic structure of the para-benzoquinone radical anion revisited. Physical Chemistry Chemical Physics, 2016, 18, 3454-3462.	2.8	14
16	Barrierless proton transfer across weak CHâ‹¯O hydrogen bonds in dimethyl ether dimer. Journal of Chemical Physics, 2015, 142, 114303.	3.0	28
17	The effects of resonance delocalization and the extent of Ï€ system on ionization energies of model fluorescent proteins chromophores. International Journal of Quantum Chemistry, 2015, 115, 1258-1264.	2.0	7
18	First-Principles Calculations of the Energy and Width of the ²A_u Shape Resonance in p-Benzoquinone: A Gateway State for Electron Transfer. Journal of Physical Chemistry Letters, 2015, 6, 1053-1058.	4.6	32

#	Article	IF	Citations
19	Role of Zwitterions in Kindling Fluorescent Protein Photochemistry. Journal of Physical Chemistry B, 2015, 119, 2467-2474.	2.6	8
20	Advances in molecular quantum chemistry contained in the Q-Chem 4 program package. Molecular Physics, 2015, 113, 184-215.	1.7	2,561
21	A Fresh Look at Resonances and Complex Absorbing Potentials: Density Matrix-Based Approach. Journal of Physical Chemistry Letters, 2014, 5, 310-315.	4.6	99
22	Complex absorbing potentials within EOM-CC family of methods: Theory, implementation, and benchmarks. Journal of Chemical Physics, 2014, 141, 024102.	3.0	113
23	Chromophore Photoreduction in Red Fluorescent Proteins Is Responsible for Bleaching and Phototoxicity. Journal of Physical Chemistry B, 2014, 118, 4527-4534.	2.6	55
24	Proton Transfer in Nucleobases is Mediated by Water. Journal of Physical Chemistry A, 2013, 117, 6789-6797.	2.5	43
25	Complex-scaled equation-of-motion coupled-cluster method with single and double substitutions for autoionizing excited states: Theory, implementation, and examples. Journal of Chemical Physics, 2013, 138, 124106.	3.0	63
26	On the Photodetachment from the Green Fluorescent Protein Chromophore. Journal of Physical Chemistry A, 2013, 117, 11815-11822.	2.5	34
27	Four Bases Score a Run: Ab Initio Calculations Quantify a Cooperative Effect of H-Bonding and Ï€-Stacking on the Ionization Energy of Adenine in the AATT Tetramer. Journal of Physical Chemistry Letters, 2012, 3, 2726-2732.	4.6	43
28	Ionization of dimethyluracil dimers leads to facile proton transfer in the absence of hydrogen bonds. Nature Chemistry, 2012, 4, 323-329.	13.6	69
29	Quantum Chemistry Behind Bioimaging: Insights from Ab Initio Studies of Fluorescent Proteins and Their Chromophores. Accounts of Chemical Research, 2012, 45, 265-275.	15.6	125
30	Insight into the Common Mechanism of the Chromophore Formation in the Red Fluorescent Proteins: The Elusive Blue Intermediate Revealed. Journal of the American Chemical Society, 2012, 134, 2807-2814.	13.7	38
31	Toward Molecular-Level Characterization of Photoinduced Decarboxylation of the Green Fluorescent Protein: Accessibility of the Charge-Transfer States. Journal of Chemical Theory and Computation, 2012, 8, 1912-1920.	5.3	25
32	The effect of microhydration on ionization energies of thymine. Faraday Discussions, 2011, 150, 313.	3.2	38
33	Effect of Protein Environment on Electronically Excited and Ionized States of the Green Fluorescent Protein Chromophore. Journal of Physical Chemistry B, 2011, 115, 8296-8303.	2.6	87
34	Effect of microhydration on the electronic structure of the chromophores of the photoactive yellow and green fluorescent proteins. Journal of Chemical Physics, 2011, 135, 194304.	3.0	31
35	The effect of Ï€-stacking, H-bonding, and electrostatic interactions on the ionization energies of nucleic acid bases: adenineâ€“adenine, thymineâ€“thymine and adenineâ€“thymine dimers. Physical Chemistry Chemical Physics, 2010, 12, 2292.	2.8	88
36	Electronic Structure and Spectroscopy of Nucleic Acid Bases: Ionization Energies, Ionization-Induced Structural Changes, and Photoelectron Spectra. Journal of Physical Chemistry A, 2010, 114, 12305-12317.	2.5	91

#	Article	IF	Citations
37	Ionization of cytosine monomer and dimer studied by VUV photoionization and electronic structure calculations. Physical Chemistry Chemical Physics, 2010, 12, 2860.	2.8	65
38	Gas Phase Absorption Studies of Photoactive Yellow Protein Chromophore Derivatives. Journal of Physical Chemistry A, 2009, 113, 9442-9449.	2.5	56
39	Modeling Photoabsorption of the asFP595 Chromophore. Journal of Physical Chemistry A, 2008, 112, 8804-8810.	2.5	32
40	An Opsin Shift in Rhodopsin:â€‰ Retinal S0â^'S1 Excitation in Protein, in Solution, and in the Gas Phase. Journal of the American Chemical Society, 2007, 129, 13035-13042.	13.7	94
41	Gas-Phase Spectroscopy of Protonated 3-OH Kynurenine and Argpyrimidine. Comparison of Experimental Results to Theoretical Modeling. Journal of Physical Chemistry A, 2007, 111, 10537-10543.	2.5	12
42	Accurate modeling of the S 0 -S 1 photo-absorption in biological chromophores. , 2007, , .		6
43	Molecular Modeling the Reaction Mechanism of Serine-Carboxyl Peptidases. Journal of Chemical Theory and Computation, 2006, 2, 1168-1175.	5.3	10