Luca De Vico

List of Publications by Year in descending order

45 papers	4,343 citations	304743 22 h-index	243625 44 g-index
48 all docs	48 docs citations	48 times ranked	4799 citing authors

#	Article	IF	Citations
1	MOLCAS 7: The Next Generation. Journal of Computational Chemistry, 2010, 31, 224-247.	3.3	1,485
2	<scp>Molcas</scp> 8: New capabilities for multiconfigurational quantum chemical calculations across the periodic table. Journal of Computational Chemistry, 2016, 37, 506-541.	3.3	1,317
3	Modern quantum chemistry with [Open]Molcas. Journal of Chemical Physics, 2020, 152, 214117.	3.0	281
4	Chemiluminescence of 1,2-Dioxetane. Reaction Mechanism Uncovered. Journal of Physical Chemistry A, 2007, 111, 8013-8019.	2.5	106
5	Theoretical Study of the Chemiluminescent Decomposition of Dioxetanone. Journal of the American Chemical Society, 2009, 131, 6181-6188.	13.7	98
6	New General Tools for Constrained Geometry Optimizations. Journal of Chemical Theory and Computation, 2005, 1, 1029-1037.	5.3	94
7	A Fast Photoswitch for Minimally Perturbed Peptides:Â Investigation of the trans â†' cis Photoisomerization ofN-Methylthioacetamide. Journal of the American Chemical Society, 2004, 126, 8823-8834.	13.7	79
8	Reaction Path Analysis of the â€œTunableâ€•Photoisomerization Selectivity of Free and Locked Retinal Chromophores. Journal of the American Chemical Society, 2002, 124, 4124-4134.	13.7	68
9	Ab initio investigation on the chemical origin of the firefly bioluminescence. Journal of Photochemistry and Photobiology A: Chemistry, 2008, 194, 261-267.	3.9	57
10	A theoretical study of singlet low-energy excited states of the benzene dimer. Chemical Physics Letters, 2006, 426, 268-272.	2.6	52
11	A CASSCF/CASPT2 approach to the decomposition of thiazole-substituted dioxetanone: Substitution effects and charge-transfer induced electron excitation. Chemical Physics Letters, 2009, 484, 69-75.	2.6	52
12	a-ARM: Automatic Rhodopsin Modeling with Chromophore Cavity Generation, Ionization State Selection, and External Counterion Placement. Journal of Chemical Theory and Computation, 2019, 15, 3134-3152.	5.3	44
13	Characterization of the conical intersection of the visual pigment rhodopsin at the CASPT2//CASSCF/AMBER level of theory. Molecular Physics, 2006, 104, 983-991.	1.7	43
14	Effects of buffer composition and dilution on nanowire field-effect biosensors. Nanotechnology, 2013, 24, 035501.	2.6	41
15	Quantifying signal changes in nano-wire based biosensors. Nanoscale, 2011, 3, 706-717.	5.6	37
16	Predicting and rationalizing the effect of surface charge distribution and orientation on nano-wire based FET bio-sensors. Nanoscale, 2011, 3, 3635.	5.6	35
17	Multireference Excitation Energies for Bacteriochlorophylls A within Light Harvesting System 2. Journal of Chemical Theory and Computation, 2016, 12, 1305-1313.	5.3	32
18	Azadioxatriangulenium and Diazaoxatriangulenium: Quantum Yields and Fundamental Photophysical Properties. ACS Omega, 2017, 2, 193-203.	3.5	29

#	Article	IF	Citations
19	Photoisomerization Mechanism of 11-cis-Locked Artificial Retinal Chromophores:Â Acceleration and Primary Photoproduct Assignment. Journal of the American Chemical Society, 2005, 127, 2433-2442.	13.7	27
20	Absorption and Fluorescence Lineshape Theory for Polynomial Potentials. Journal of Chemical Theory and Computation, 2016, 12, 5979-5989.	5.3	27
21	Frontiers in Multiscale Modeling of Photoreceptor Proteins. Photochemistry and Photobiology, 2021, 97, 243-269.	2.5	26
22	Photoisomerization acceleration in retinal protonated Schiff-base models. Photochemical and Photobiological Sciences, 2003, 2, 1250.	2.9	25
23	Spin-Orbit Ab Initio Investigation of the Ultraviolet Photolysis of Diiodomethane. ChemPhysChem, 2007, 8, 890-898.	2.1	25
24	Indium arsenide nanowire field-effect transistors for pH and biological sensing. Applied Physics Letters, 2014, 104, .	3.3	22
25	Macrocycle ring deformation as the secondary design principle for light-harvesting complexes. Proceedings of the National Academy of Sciences of the United States of America, 2018, 115, E9051-E9057.	7.1	21
26	Single-molecule force-conductance spectroscopy of hydrogen-bonded complexes. Journal of Chemical Physics, 2017, 146, 092329.	3.0	20
27	Intermolecular Modes between LH2 Bacteriochlorophylls and Protein Residues: The Effect on the Excitation Energies. Journal of Physical Chemistry B, 2017, 121, 5499-5508.	2.6	19
28	The ozone ring closure as a test for multi-state multi-configurational second order perturbation theory (MS-CASPT2). Chemical Physics Letters, 2008, 461, 136-141.	2.6	18
29	Assessment of MC-PDFT Excitation Energies for a Set of QM/MM Models of Rhodopsins. Journal of Chemical Theory and Computation, 2019, 15, 1915-1923.	5.3	16
30	A Computational Methodology to Screen Activities of Enzyme Variants. PLoS ONE, 2012, 7, e49849.	2.5	15
31	Q_y and Q_x Absorption Bands for Bacteriochlorophyll a Molecules from LH2 and LH3. Journal of Physical Chemistry A, 2019, 123, 5283-5292.	2.5	15
32	Two-State, Three-Mode Parametrization of the Force Field of a Retinal Chromophore Model. Journal of Physical Chemistry A, 2019, 123, 1710-1719.	2.5	15
33	Web-ARM: A Web-Based Interface for the Automatic Construction of QM/MM Models of Rhodopsins. Journal of Chemical Information and Modeling, 2020, 60, 1481-1493.	5.4	15
34	In Silico Prediction of Mutant HIV-1 Proteases Cleaving a Target Sequence. PLoS ONE, 2014, 9, e95833.	2.5	12
35	Toward a computational photobiology. Pure and Applied Chemistry, 2005, 77, 977-993.	1.9	10
36	BioFET-SIM Web Interface: Implementation and Two Applications. PLoS ONE, 2012, 7, e45379.	2.5	10

#	Article	IF	Citations
37	Boron Subphthalocyanine Based Molecular Triad Systems for the Capture of Solar Energy. Journal of Physical Chemistry A, 2016, 120, 7694-7703.	2.5	10
38	Hypothesis onSerenoa repens(Bartram) small extract inhibition of prostatic 5Î±-reductase through anin silicoapproach on 5Î²-reductase x-ray structure. PeerJ, 2016, 4, e2698.	2.0	8
39	In silicoscreening of 393 mutants facilitates enzyme engineering of amidase activity in CalB. PeerJ, 2013, 1, e145.	2.0	7
40	A computational method for the systematic screening of reaction barriers in enzymes: searching forBacillus circulansxylanase mutants with greater activity towards a synthetic substrate. PeerJ, 2013, 1, e111.	2.0	7
41	Evolution of the Automatic Rhodopsin Modeling (ARM) Protocol. Topics in Current Chemistry, 2022, 380, 21.	5.8	7
42	Location of Two Seams in the Proximity of theC_{2v}Ï€Ï€* Minimum Energy Path of Formaldehyde. Journal of Chemical Theory and Computation, 2009, 5, 186-191.	5.3	6
43	Iron(III) complexing ability of new ligands based on natural Î³-pyrone maltol. Polyhedron, 2020, 187, 114650.	2.2	6
44	On the Automatic Construction of QM/MM Models for Biological Photoreceptors: Rhodopsins as Model Systems. Challenges and Advances in Computational Chemistry and Physics, 2021, , 1-75.	0.6	4
45	BioFET-SIM: A Tool for the Analysis and Prediction of Signal Changes in Nanowire-Based Field Effect Transistor Biosensors. Lecture Notes in Nanoscale Science and Technology, 2013, , 55-86.	0.8	0