

Eduardo M Sproviero

List of Publications by Year in descending order

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Version: 2024-02-01

20
papers

1,461
citations

623188

14
h-index

752256

20
g-index

20
all docs

20
docs citations

20
times ranked

1255
citing authors

#	ARTICLE	IF	CITATIONS
1	Quantum Mechanics/Molecular Mechanics Study of the Catalytic Cycle of Water Splitting in Photosystem II. <i>Journal of the American Chemical Society</i> , 2008, 130, 3428-3442.	6.6	345
2	Computational studies of the O ₂ -evolving complex of photosystem II and biomimetic oxomanganese complexes. <i>Coordination Chemistry Reviews</i> , 2008, 252, 395-415.	9.5	146
3	QM/MM Models of the O ₂ -Evolving Complex of Photosystem II. <i>Journal of Chemical Theory and Computation</i> , 2006, 2, 1119-1134.	2.3	136
4	A Model of the Oxygen-Evolving Center of Photosystem II Predicted by Structural Refinement Based on EXAFS Simulations. <i>Journal of the American Chemical Society</i> , 2008, 130, 6728-6730.	6.6	110
5	Density Functional Theory and DFT+U Study of Transition Metal Porphines Adsorbed on Au(111) Surfaces and Effects of Applied Electric Fields. <i>Journal of the American Chemical Society</i> , 2006, 128, 3659-3668.	6.6	100
6	Characterization of synthetic oxomanganese complexes and the inorganic core of the O ₂ -evolving complex in photosystem II: Evaluation of the DFT/B3LYP level of theory. <i>Journal of Inorganic Biochemistry</i> , 2006, 100, 786-800.	1.5	99
7	Quantum mechanics/molecular mechanics structural models of the oxygen-evolving complex of photosystem II. <i>Current Opinion in Structural Biology</i> , 2007, 17, 173-180.	2.6	91
8	Deposition of an oxomanganese water oxidation catalyst on TiO ₂ nanoparticles: computational modeling, assembly and characterization. <i>Energy and Environmental Science</i> , 2009, 2, 230.	15.6	80
9	Computational Studies of the Primary Phototransduction Event in Visual Rhodopsin. <i>Accounts of Chemical Research</i> , 2006, 39, 184-193.	7.6	75
10	QM/MM computational studies of substrate water binding to the oxygen-evolving centre of photosystem II. <i>Philosophical Transactions of the Royal Society B: Biological Sciences</i> , 2008, 363, 1149-1156.	1.8	70
11	Computational insights into the O ₂ -evolving complex of photosystem II. <i>Photosynthesis Research</i> , 2008, 97, 91-114.	1.6	62
12	QM/MM Study of the NMR Spectroscopy of the Retinyl Chromophore in Visual Rhodopsin. <i>Journal of Chemical Theory and Computation</i> , 2005, 1, 674-685.	2.3	45
13	The MoD-QM/MM methodology for structural refinement of photosystem II and other biological macromolecules. <i>Photosynthesis Research</i> , 2009, 102, 455-470.	1.6	41
14	Theoretical EXAFS studies of a model of the oxygen-evolving complex of photosystem II obtained with the quantum cluster approach. <i>International Journal of Quantum Chemistry</i> , 2013, 113, 474-478.	1.0	26
15	Stereoelectronic Contributions to Long-Range $1H\hat{\alpha}^1H$ Coupling Constants ¹ . <i>Journal of Physical Chemistry A</i> , 2002, 106, 7834-7843.	1.1	11
16	Stereoelectronic Interactions and Molecular Properties. An NBO-Based Study of Uracil. <i>Journal of Physical Chemistry A</i> , 2003, 107, 5544-5554.	1.1	10
17	A DFT/B3LYP study of the mechanisms of the O ₂ formation reaction catalyzed by the [(terpy)(H ₂ O)Mn ^{III} (O) ₂ Mn ^{IV} (OH) ₂ (terpy)](NO ₃) ₃ complex: A paradigm for photosystem II. <i>Journal of Inorganic Biochemistry</i> , 2017, 171, 52-66.	1.5	7
18	Geometrical properties of the manganese(IV)/iron(III) cofactor of <i>Chlamydia trachomatis</i> ribonucleotide reductase unveiled by simulations of XAS spectra. <i>Dalton Transactions</i> , 2017, 46, 4724-4736.	1.6	3

#	ARTICLE	IF	CITATIONS
19	Opsin Effect on the Electronic Structure of the Retinylidene Chromophore in Rhodopsin. Journal of Chemical Theory and Computation, 2015, 11, 1206-1219.	2.3	2
20	Intramolecular Natural Energy Decomposition Analysis: Applications to the Rational Design of Foldamers. Journal of Computational Chemistry, 2018, 39, 1367-1386.	1.5	2