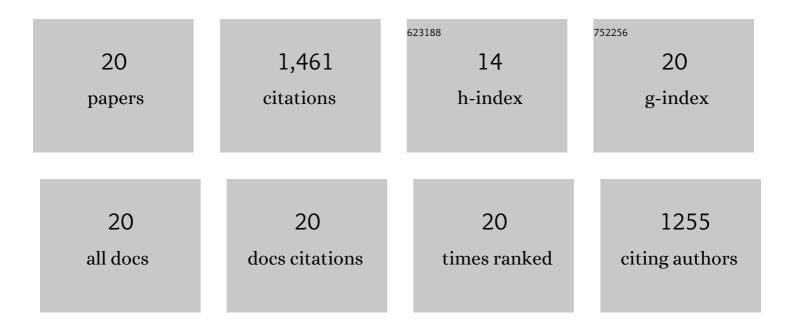
## Eduardo M Sproviero

List of Publications by Year in descending order

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#	Article	IF	CITATIONS
1	Quantum Mechanics/Molecular Mechanics Study of the Catalytic Cycle of Water Splitting in Photosystem II. Journal of the American Chemical Society, 2008, 130, 3428-3442.	6.6	345
2	Computational studies of the O2-evolving complex of photosystem II and biomimetic oxomanganese complexes. Coordination Chemistry Reviews, 2008, 252, 395-415.	9.5	146
3	QM/MM Models of the O2-Evolving Complex of Photosystem II. Journal of Chemical Theory and Computation, 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. Journal of the American Chemical Society, 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. Journal of the American Chemical Society, 2006, 128, 3659-3668.	6.6	100
6	Characterization of synthetic oxomanganese complexes and the inorganic core of the O2-evolving complex in photosystem II: Evaluation of the DFT/B3LYP level of theory. Journal of Inorganic Biochemistry, 2006, 100, 786-800.	1.5	99
7	Quantum mechanics/molecular mechanics structural models of the oxygen-evolving complex of photosystem II. Current Opinion in Structural Biology, 2007, 17, 173-180.	2.6	91
8	Deposition of an oxomanganese water oxidation catalyst on TiO2 nanoparticles: computational modeling, assembly and characterization. Energy and Environmental Science, 2009, 2, 230.	15.6	80
9	Computational Studies of the Primary Phototransduction Event in Visual Rhodopsin. Accounts of Chemical Research, 2006, 39, 184-193.	7.6	75
10	QM/MM computational studies of substrate water binding to the oxygen-evolving centre of photosystem II. Philosophical Transactions of the Royal Society B: Biological Sciences, 2008, 363, 1149-1156.	1.8	70
11	Computational insights into the O2-evolving complex of photosystem II. Photosynthesis Research, 2008, 97, 91-114.	1.6	62
12	QM/MM Study of the NMR Spectroscopy of the Retinyl Chromophore in Visual Rhodopsin. Journal of Chemical Theory and Computation, 2005, 1, 674-685.	2.3	45
13	The MoD-QM/MM methodology for structural refinement of photosystem II and other biological macromolecules. Photosynthesis Research, 2009, 102, 455-470.	1.6	41
14	Theoretical EXAFS studies of a model of the oxygenâ€evolving complex of photosystem II obtained with the quantum cluster approach. International Journal of Quantum Chemistry, 2013, 113, 474-478.	1.0	26
15	Stereoelectronic Contributions to Long-Range1Hâ^'1H Coupling Constants1. Journal of Physical Chemistry A, 2002, 106, 7834-7843.	1.1	11
16	Stereoelectronic Interactions and Molecular Properties. An NBO-Based Study of Uracil. Journal of Physical Chemistry A, 2003, 107, 5544-5554.	1.1	10
17	A DFT/B3LYP study of the mechanisms of the O2 formation reaction catalyzed by the [(terpy)(H2O)MnIII(O)2MnIV(OH2)(terpy)](NO3)3 complex: A paradigm for photosystem II. Journal of Inorganic Biochemistry, 2017, 171, 52-66.	1.5	7
18	Geometrical properties of the manganese(iv)/iron(iii) cofactor of Chlamydia trachomatis ribonucleotide reductase unveiled by simulations of XAS spectra. Dalton Transactions, 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