Agostino Migliore

List of Publications by Year
in descending order

40 papers	2,308 citations	394421 19 h-index	302126 39 g-index
44 all docs	44 docs citations	44 times ranked	3056 citing authors

#	Article	IF	Citations
1	Symmetry-Induced Emergence of a Pseudo-Qutrit in the Dipolar Coupling of Two Qubits. Entropy, 2022, 24, 223.	2.2	2
2	Temperature Dependence of Charge and Spin Transfer in Azurin. Journal of Physical Chemistry C, 2021, 125, 9875-9883.	3.1	26
3	The physical origin of a photon-number parity effect in cavity quantum electrodynamics. Results in Physics, 2021, 30, 104690.	4.1	4
4	New approach to describe two coupled spins in a variable magnetic field. AIP Conference Proceedings, 2021, , .	0.4	3
5	Correlation between Charge Transport and Base Excision Repair in the MutYâ€“DNA Glycosylase. Journal of Physical Chemistry B, 2021, 125, 17-23.	2.6	4
6	Mechanism of Side Chain-Controlled Proton Conductivity in Bioinspired Peptidic Nanostructures. Journal of Physical Chemistry B, 2021, 125, 12741-12752.	2.6	3
7	Mutation effects on charge transport through the p58c ironâ€“sulfur protein. Chemical Science, 2020, 11, 7076-7085.	7.4	5
8	Electrostatic Field-Induced Oscillator Strength Focusing in Molecules. Journal of Physical Chemistry B, 2020, 124, 6376-6388.	2.6	5
9	Mapping hole hopping escape routes in proteins. Proceedings of the National Academy of Sciences of the United States of America, 2019, 116, 15811-15816.	7.1	35
10	How To Extract Quantitative Information on Electronic Transitions from the Density Functional Theory â€œBlack Boxâ€• Journal of Chemical Theory and Computation, 2019, 15, 4915-4923.	5.3	9
11	A single ATâ€“GC exchange can modulate charge transfer-induced p53â€“DNA dissociation. Chemical Communications, 2019, 55, 206-209.	4.1	11
12	2â€²-Deoxy-2â€²-fluoro-arabinonucleic acid: a valid alternative to DNA for biotechnological applications using charge transport. Physical Chemistry Chemical Physics, 2019, 21, 22869-22878.	2.8	6
13	Charge Transfer between [4Fe4S] Proteins and DNA Is Unidirectional: Implications for Biomolecular Signaling. CheM, 2019, 5, 122-137.	11.7	25
14	Determinants of Photolyaseâ€™s DNA Repair Mechanism in Mesophiles and Extremophiles. Journal of the American Chemical Society, 2018, 140, 2853-2861.	13.7	19
15	Electron transfer characteristics of 2â€²-deoxy-2â€²-fluoro-arabinonucleic acid, a nucleic acid with enhanced chemical stability. Physical Chemistry Chemical Physics, 2018, 20, 26063-26067.	2.8	8
16	Covalently bonded single-molecule junctions with stable and reversible photoswitched conductivity. Science, 2016, 352, 1443-1445.	12.6	697
17	Where Is the Electronic Oscillator Strength? Mapping Oscillator Strength across Molecular Absorption Spectra. Journal of Physical Chemistry A, 2016, 120, 1933-1943.	2.5	38
18	DNA from First Principles. , 2016, , 800-819.		0

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19	Irreversibility in redox molecular conduction: single versus double metal-molecule interfaces. Electrochimica Acta, 2015, 160, 363-375.	5.2	13
20	Sensing of molecules using quantum dynamics. Proceedings of the National Academy of Sciences of the United States of America, 2015, 112, E2419-28.	7.1	14
21	Defusing redox bombs?. Proceedings of the National Academy of Sciences of the United States of America, 2015, 112, 10821-10822.	7.1	30
22	Charge Transfer in Dynamical Biosystems, or The Treachery of (Static) Images. Accounts of Chemical Research, 2015, 48, 474-481.	15.6	145
23	Cu-To-Cu Electron Tunneling in Copper Monooxygenases. Biophysical Journal, 2014, 106, 588a.	0.5	0
24	Long-range charge transport in single G-quadruplex DNA molecules. Nature Nanotechnology, 2014, 9, 1040-1046.	31.5	218
25	Biochemistry and Theory of Proton-Coupled Electron Transfer. Chemical Reviews, 2014, 114, 3381-3465.	47.7	399
26	Dynamical Treatment of Charge Transfer through Duplex Nucleic Acids Containing Modified Adenines. ACS Nano, 2013, 7, 9396-9406.	14.6	8
27	Irreversibility and Hysteresis in Redox Molecular Conduction Junctions. Journal of the American Chemical Society, 2013, 135, 9420-9432.	13.7	62
28	Quantum transport with two interacting conduction channels. Journal of Chemical Physics, 2013, 138, 174111.	3.0	14
29	On the relationship between molecular state and single electron pictures in simple electrochemical junctions. Physical Chemistry Chemical Physics, 2012, 14, 13746.	2.8	59
30	On the evaluation of the Marcusâ€“Hushâ€“Chidsey integral. Journal of Electroanalytical Chemistry, 2012, 671, 99-101.	3.8	24
31	Nonorthogonality Problem and Effective Electronic Coupling Calculation: Application to Charge Transfer in Ï€-Stacks Relevant to Biochemistry and Molecular Electronics. Journal of Chemical Theory and Computation, 2011, 7, 1712-1725.	5.3	52
32	Nonlinear Charge Transport in Redox Molecular Junctions: A Marcus Perspective. ACS Nano, 2011, 5, 6669-6685.	14.6	111
33	Quantum Mechanical and Quantum Mechanical/Molecular Mechanical Studies of the Ironâ^'Dioxygen Intermediates and Proton Transfer in Superoxide Reductase. Journal of Chemical Theory and Computation, 2010, 6, 2896-2909.	5.3	19
34	Full-electron calculation of effective electronic couplings and excitation energies of charge transfer states: Application to hole transfer in DNA Ï€-stacks. Journal of Chemical Physics, 2009, 131, 114113.	3.0	33
35	Evaluation of Electronic Coupling in Transition-Metal Systems Using DFT: Application to the Hexa-Aquo Ferricâ^'Ferrous Redox Couple. Journal of Chemical Theory and Computation, 2009, 5, 307-323.	5.3	41
36	Ab initio Study of the Structural, Tautomeric, Pairing, and Electronic Properties of Seleno-Derivatives of Thymine. Journal of Physical Chemistry B, 2009, 113, 14465-14472.	2.6	15

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37	First Principles Effective Electronic Couplings for Hole Transfer in Natural and Size-Expanded DNA. Journal of Physical Chemistry B, 2009, 113, 9402-9415.	2.6	64
38	Water-Mediated Electron Transfer between Protein Redox Centers. Journal of Physical Chemistry B, 2007, 111, 3774-3781.	2.6	27
39	First-principles density-functional theory calculations of electron-transfer rates in azurin dimers. Journal of Chemical Physics, 2006, 124, 064501.	3.0	42
40	Water Effects on Electron Transfer in Azurin Dimers. Journal of Physical Chemistry B, 2006, 110, 23796-23800.	2.6	16