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	Covalently bonded single-molecule junctions with stable and reversible photoswitched conductivity. Science, 2016, 352, 1443-1445.	12.6	697
2	Biochemistry and Theory of Proton-Coupled Electron Transfer. Chemical Reviews, 2014, 114, 3381-3465.	47.7	399
3	Long-range charge transport in single G-quadruplex DNA molecules. Nature Nanotechnology, 2014, 9, 1040-1046.	31.5	218
4	Charge Transfer in Dynamical Biosystems, or The Treachery of (Static) Images. Accounts of Chemical Research, 2015, 48, 474-481.	15.6	145
5	Nonlinear Charge Transport in Redox Molecular Junctions: A Marcus Perspective. ACS Nano, 2011, 5, 6669-6685.	14.6	111
6	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
7	Irreversibility and Hysteresis in Redox Molecular Conduction Junctions. Journal of the American Chemical Society, 2013, 135, 9420-9432.	13.7	62
8	On the relationship between molecular state and single electron pictures in simple electrochemical junctions. Physical Chemistry Chemical Physics, 2012, 14, 13746.	2.8	59
9	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
10	First-principles density-functional theory calculations of electron-transfer rates in azurin dimers. Journal of Chemical Physics, 2006, 124, 064501.	3.0	42
11	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
12	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
13	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
14	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
15	Defusing redox bombs?. Proceedings of the National Academy of Sciences of the United States of America, 2015, 112, 10821-10822.	7.1	30
16	Water-Mediated Electron Transfer between Protein Redox Centers. Journal of Physical Chemistry B, 2007, 111, 3774-3781.	2.6	27
17	Temperature Dependence of Charge and Spin Transfer in Azurin. Journal of Physical Chemistry C, 2021, 125, 9875-9883.	3.1	26
18	Charge Transfer between [4Fe4S] Proteins and DNA Is Unidirectional: Implications for Biomolecular Signaling. CheM, 2019, 5, 122-137.	11.7	25

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19	On the evaluation of the Marcusâ€“Hushâ€“Chidsey integral. Journal of Electroanalytical Chemistry, 2012, 671, 99-101.	3.8	24
20	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
21	Determinants of Photolyaseâ€™s DNA Repair Mechanism in Mesophiles and Extremophiles. Journal of the American Chemical Society, 2018, 140, 2853-2861.	13.7	19
22	Water Effects on Electron Transfer in Azurin Dimers. Journal of Physical Chemistry B, 2006, 110, 23796-23800.	2.6	16
23	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
24	Quantum transport with two interacting conduction channels. Journal of Chemical Physics, 2013, 138, 174111.	3.0	14
25	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
26	Irreversibility in redox molecular conduction: single versus double metal-molecule interfaces. Electrochimica Acta, 2015, 160, 363-375.	5.2	13
27	A single ATâ€“GC exchange can modulate charge transfer-induced p53â€“DNA dissociation. Chemical Communications, 2019, 55, 206-209.	4.1	11
28	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
29	Dynamical Treatment of Charge Transfer through Duplex Nucleic Acids Containing Modified Adenines. ACS Nano, 2013, 7, 9396-9406.	14.6	8
30	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
31	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
32	Mutation effects on charge transport through the p58c ironâ€“sulfur protein. Chemical Science, 2020, 11, 7076-7085.	7.4	5
33	Electrostatic Field-Induced Oscillator Strength Focusing in Molecules. Journal of Physical Chemistry B, 2020, 124, 6376-6388.	2.6	5
34	The physical origin of a photon-number parity effect in cavity quantum electrodynamics. Results in Physics, 2021, 30, 104690.	4.1	4
35	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
36	New approach to describe two coupled spins in a variable magnetic field. AIP Conference Proceedings, 2021, , .	0.4	3

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37	Mechanism of Side Chain-Controlled Proton Conductivity in Bioinspired Peptidic Nanostructures. Journal of Physical Chemistry B, 2021, 125, 12741-12752.	2.6	3
38	Symmetry-Induced Emergence of a Pseudo-Qutrit in the Dipolar Coupling of Two Qubits. Entropy, 2022, 24, 223.	2.2	2
39	Cu-To-Cu Electron Tunneling in Copper Monooxygenases. Biophysical Journal, 2014, 106, 588a.	0.5	0
40	DNA from First Principles. , 2016, , 800-819.		0