

Giuliano Mallocci

List of Publications by Year in descending order

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92
papers

2,434
citations

159358

30
h-index

233125

45
g-index

95
all docs

95
docs citations

95
times ranked

2655
citing authors

#	ARTICLE	IF	CITATIONS
1	On-line database of the spectral properties of polycyclic aromatic hydrocarbons. <i>Chemical Physics</i> , 2007, 332, 353-359.	0.9	164
2	Electronic and optical properties of families of polycyclic aromatic hydrocarbons: A systematic (time-dependent) density functional theory study. <i>Chemical Physics</i> , 2011, 384, 19-27.	0.9	139
3	Electronic absorption spectra of PAHs up to vacuum UV. <i>Astronomy and Astrophysics</i> , 2004, 426, 105-117.	2.1	112
4	Time-dependent density functional study of the electronic spectra of oligoacenes in the charge states $\tilde{n}^1, 0, +1$, and $+2$. <i>Chemical Physics</i> , 2007, 340, 43-58.	0.9	100
5	Bacterial Outer Membrane Porins as Electrostatic Nanosieves: Exploring Transport Rules of Small Polar Molecules. <i>ACS Nano</i> , 2017, 11, 5465-5473.	7.3	74
6	The complex of ferric-enterobactin with its transporter from <i>Pseudomonas aeruginosa</i> suggests a two-site model. <i>Nature Communications</i> , 2019, 10, 3673.	5.8	62
7	Theoretical evaluation of PAH dication properties. <i>Astronomy and Astrophysics</i> , 2007, 462, 627-635.	2.1	61
8	Molecular Rationale behind the Differential Substrate Specificity of Bacterial RND Multi-Drug Transporters. <i>Scientific Reports</i> , 2017, 7, 8075.	1.6	58
9	Theoretical electron affinities of PAHs and electronic absorption spectra of their mono-anions. <i>Astronomy and Astrophysics</i> , 2005, 432, 585-594.	2.1	57
10	High-resolution infrared absorption spectroscopy of thermally excited naphthalene. Measurements and calculations of anharmonic parameters and vibrational interactions. <i>Physical Chemistry Chemical Physics</i> , 2009, 11, 3443.	1.3	57
11	The role of the charge state of PAHs in ultraviolet extinction. <i>Astronomy and Astrophysics</i> , 2008, 486, L25-L29.	2.1	54
12	Chlorpromazine and Amitriptyline Are Substrates and Inhibitors of the AcrB Multidrug Efflux Pump. <i>MBio</i> , 2020, 11, .	1.8	54
13	A general model for the identification of specific PAHs in the far-IR. <i>Astronomy and Astrophysics</i> , 2006, 460, 93-104.	2.1	53
14	A Database of Force-Field Parameters, Dynamics, and Properties of Antimicrobial Compounds. <i>Molecules</i> , 2015, 20, 13997-14021.	1.7	48
15	Effects of TIPS-Functionalization and Perhalogenation on the Electronic, Optical, and Transport Properties of Angular and Compact Dibenzochrysene. <i>Journal of Physical Chemistry A</i> , 2014, 118, 5170-5177.	1.1	46
16	Dehydrogenated polycyclic aromatic hydrocarbons and UV bump. <i>Astronomy and Astrophysics</i> , 2008, 489, 1183-1187.	2.1	44
17	Diagnostics for specific PAHs in the far-IR: searching neutral naphthalene and anthracene in the Red Rectangle. <i>Astronomy and Astrophysics</i> , 2006, 456, 161-169.	2.1	42
18	The effect of selective interactions at the interface of polymer-oxide hybrid solar cells. <i>Energy and Environmental Science</i> , 2012, 5, 9068.	15.6	42

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19	Interfacial Engineering of P3HT/ZnO Hybrid Solar Cells Using Phthalocyanines: A Joint Theoretical and Experimental Investigation. <i>Advanced Energy Materials</i> , 2014, 4, 1301694.	10.2	42
20	Water-mediated interactions enable smooth substrate transport in a bacterial efflux pump. <i>Biochimica Et Biophysica Acta - General Subjects</i> , 2018, 1862, 836-845.	1.1	42
21	Structural and Optoelectronic Properties of Unsaturated ZnO and ZnS Nanoclusters. <i>Journal of Physical Chemistry C</i> , 2012, 116, 8741-8746.	1.5	41
22	Visible photodissociation spectroscopy of PAH cations and derivatives in the PIRENEA experiment. <i>Chemical Physics</i> , 2010, 371, 16-23.	0.9	40
23	Search for corannulene (C ₂₀ H ₁₀) in the Red Rectangle. <i>Monthly Notices of the Royal Astronomical Society</i> , 2009, 397, 1053-1060.	1.6	39
24	Molecular Determinants of the Promiscuity of MexB and MexY Multidrug Transporters of <i>Pseudomonas aeruginosa</i> . <i>Frontiers in Microbiology</i> , 2018, 9, 1144.	1.5	37
25	Binding and Transport of Carboxylated Drugs by the Multidrug Transporter AcrB. <i>Journal of Molecular Biology</i> , 2020, 432, 861-877.	2.0	37
26	Zinc Oxideâ€Zinc Phthalocyanine Interface for Hybrid Solar Cells. <i>Journal of Physical Chemistry C</i> , 2012, 116, 15439-15448.	1.5	36
27	Perturbed structural dynamics underlie inhibition and altered efflux of the multidrug resistance pump AcrB. <i>Nature Communications</i> , 2020, 11, 5565.	5.8	34
28	The challenge of intracellular antibiotic accumulation, a function of fluoroquinolone influx versus bacterial efflux. <i>Communications Biology</i> , 2020, 3, 198.	2.0	34
29	Electronic excitations of oligoacenes: A time dependent density functional theory study. <i>Superlattices and Microstructures</i> , 2009, 46, 14-18.	1.4	33
30	Holo-like and Druggable Protein Conformations from Enhanced Sampling of Binding Pocket Volume and Shape. <i>Journal of Chemical Information and Modeling</i> , 2019, 59, 1515-1528.	2.5	33
31	Estimated IR and phosphorescence emission fluxes for specific polycyclic aromatic hydrocarbons in the Red Rectangle. <i>Astronomy and Astrophysics</i> , 2006, 446, 537-549.	2.1	32
32	Computer simulations of the activity of RND efflux pumps. <i>Research in Microbiology</i> , 2018, 169, 384-392.	1.0	32
33	Efficient calculation of van der Waals dispersion coefficients with time-dependent density functional theory in real time: Application to polycyclic aromatic hydrocarbons. <i>Journal of Chemical Physics</i> , 2007, 127, 014107.	1.2	31
34	Computational modelling of efflux pumps and their inhibitors. <i>Essays in Biochemistry</i> , 2017, 61, 141-156.	2.1	31
35	Polymer Crystallinity and Transport Properties at the Poly(3-hexylthiophene)/Zinc Oxide Interface. <i>Journal of Physical Chemistry C</i> , 2011, 115, 9651-9655.	1.5	30
36	Electronic and optical properties of hexathiapentacene in the gas and crystal phases. <i>Physical Review B</i> , 2016, 93, .	1.1	29

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37	Predictive Rules of Efflux Inhibition and Avoidance in <i>Pseudomonas aeruginosa</i> . <i>MBio</i> , 2021, 12, .	1.8	28
38	Pyridylpiperazine-based allosteric inhibitors of RND-type multidrug efflux pumps. <i>Nature Communications</i> , 2022, 13, 115.	5.8	28
39	A New Critical Conformational Determinant of Multidrug Efflux by an MFS Transporter. <i>Journal of Molecular Biology</i> , 2018, 430, 1368-1385.	2.0	27
40	Structural and functional analysis of the promiscuous AcrB and AdeB efflux pumps suggests different drug binding mechanisms. <i>Nature Communications</i> , 2021, 12, 6919.	5.8	25
41	Quasiparticle effects and optical absorption in small fullerene-like GaP clusters. <i>Physical Review B</i> , 2004, 70, .	1.1	24
42	Bacterial efflux transporters'™ polyspecificity " a gift and a curse?. <i>Current Opinion in Microbiology</i> , 2021, 61, 115-123.	2.3	23
43	Rationalizing the permeation of polar antibiotics into Gram-negative bacteria. <i>Journal of Physics Condensed Matter</i> , 2017, 29, 113001.	0.7	22
44	Testing the "strong"•PAHs hypothesis. <i>Astronomy and Astrophysics</i> , 2003, 410, 639-648.	2.1	22
45	Testing the "strong"•PAHs hypothesis. <i>Astronomy and Astrophysics</i> , 2003, 410, 623-637.	2.1	21
46	Tuning Optical Properties of Dibenzochrysenes by Functionalization: A Many-Body Perturbation Theory Study. <i>Journal of Physical Chemistry C</i> , 2017, 121, 24480-24488.	1.5	18
47	Molecular Interactions of Cephalosporins with the Deep Binding Pocket of the RND Transporter AcrB. <i>Journal of Physical Chemistry B</i> , 2019, 123, 4625-4635.	1.2	18
48	Identification and characterization of carbapenem binding sites within the RND-transporter AcrB. <i>Biochimica Et Biophysica Acta - Biomembranes</i> , 2019, 1861, 62-74.	1.4	18
49	Electronic Properties and Quantum Confinement in Bi ₂ S ₃ Ribbon-Like Nanostructures. <i>Journal of Physical Chemistry C</i> , 2013, 117, 21923-21929.	1.5	17
50	Extracting Conformational Ensembles of Small Molecules from Molecular Dynamics Simulations: Ampicillin as a Test Case. <i>Computation</i> , 2016, 4, 5.	1.0	17
51	Exploiting the porin pathway for polar compound delivery into Gram-negative bacteria. <i>Future Medicinal Chemistry</i> , 2016, 8, 1047-1062.	1.1	16
52	Mechanistic Duality of Bacterial Efflux Substrates and Inhibitors: Example of Simple Substituted Cinnamoyl and Naphthyl Amides. <i>ACS Infectious Diseases</i> , 2021, 7, 2650-2665.	1.8	16
53	Large prebiotic molecules in space: photophysics of acetic acid and its isomers. <i>Monthly Notices of the Royal Astronomical Society</i> , 2010, 402, 1667-1674.	1.6	14
54	Optoelectronic properties of (ZnO) ₆₀ isomers. <i>Physical Chemistry Chemical Physics</i> , 2012, 14, 14293.	1.3	14

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55	Electronic Properties of Hybrid Zinc Oxideâ€“Oligothiophene Nanostructures. <i>Journal of Physical Chemistry C</i> , 2012, 116, 8174-8180.	1.5	13
56	Role of Molecular Thermodynamical Processes at Functionalized Polymer/Metaloxide Interfaces for Photovoltaics. <i>Journal of Physical Chemistry C</i> , 2013, 117, 13894-13901.	1.5	13
57	Computational investigation of the effects of perfluorination on the charge-transport properties of polyaromatic hydrocarbons. <i>Chemical Physics</i> , 2016, 478, 8-13.	0.9	13
58	Coupling enhanced sampling of the apo-receptor with template-based ligand conformers selection: performance in pose prediction in the D3R Grand Challenge 4. <i>Journal of Computer-Aided Molecular Design</i> , 2020, 34, 149-162.	1.3	11
59	Molecular Interactions of Carbapenem Antibiotics with the Multidrug Efflux Transporter AcrB of <i>Escherichia coli</i> . <i>International Journal of Molecular Sciences</i> , 2020, 21, 860.	1.8	11
60	Search for far-IR PAH bands with Herschel: modelling and observational approaches. <i>EAS Publications Series</i> , 2011, 46, 123-130.	0.3	10
61	A (time-dependent) density functional theory study of the optoelectronic properties of bis-triisopropylsilylethynyl-functionalized acenes. <i>Thin Solid Films</i> , 2013, 543, 32-34.	0.8	10
62	Recognition of quinolone antibiotics by the multidrug efflux transporter MexB of <i>Pseudomonas aeruginosa</i> . <i>Physical Chemistry Chemical Physics</i> , 2022, 24, 16566-16575.	1.3	9
63	Complexes formed by the siderophore-based monosulfactam antibiotic BAL30072 and their interaction with the outer membrane receptor PiuA of <i>P. aeruginosa</i> . <i>BioMetals</i> , 2019, 32, 155-170.	1.8	8
64	Time-Dependent Density Functional Theory Investigation on the Electronic and Optical Properties of Poly-C,Si,Ge-acenes. <i>ACS Omega</i> , 2020, 5, 16654-16663.	1.6	8
65	Multidrug Efflux Pumps and Their Inhibitors Characterized by Computational Modeling. , 2016, , 797-831.		7
66	Molecular Modeling of Multidrug Properties of Resistance Nodulation Division (RND) Transporters. <i>Methods in Molecular Biology</i> , 2018, 1700, 179-219.	0.4	6
67	Modelling photoluminescence from small particles. <i>Astronomy and Astrophysics</i> , 2004, 420, 921-927.	2.1	6
68	AB-DB: Force-Field parameters, MD trajectories, QM-based data, and Descriptors of Antimicrobials. <i>Scientific Data</i> , 2022, 9, 148.	2.4	6
69	Modelling photoluminescence from small particles. <i>Astronomy and Astrophysics</i> , 2004, 420, 809-820.	2.1	5
70	Modelling peculiar extinction curves. <i>Monthly Notices of the Royal Astronomical Society</i> , 2010, , no-no.	1.6	5
71	Electronic and optical properties of functionalized polyaromatic hydrocarbons: a computational investigation on perfluorinated circumacenes. <i>Proceedings of SPIE</i> , 2016, , .	0.8	4
72	Molecular rationale for the impairment of the MexAB-OprM efflux pump by a single mutation in MexA. <i>Computational and Structural Biotechnology Journal</i> , 2022, 20, 252-260.	1.9	4

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73	Theoretical spectral properties of PAHs: towards a detailed model of their photophysics in the ISM. Journal of Physics: Conference Series, 2005, 6, 178-184.	0.3	3
74	Selective Synthesis of α -Sulfonyl Carbonyl Compounds from Internal Alkynes and Thiols via Photoredox Catalysis. Advanced Synthesis and Catalysis, 0, , .	2.1	3
75	Polycyclic Aromatic Hydrocarbons and the Extinction Curve. EAS Publications Series, 2011, 46, 327-340.	0.3	2
76	Molecular insights into the Patched1 drug efflux inhibitory activity of panicein A hydroquinone: a computational study. Physical Chemistry Chemical Physics, 2021, 23, 8013-8022.	1.3	2
77	Inhibition of the drug efflux activity of Ptch1 as a promising strategy to overcome chemotherapy resistance in cancer cells. European Journal of Medicinal Chemistry, 2022, 236, 114306.	2.6	2
78	Identifying specific interstellar polycyclic aromatic hydrocarbons. Journal of Physics: Conference Series, 2005, 6, 217-222.	0.3	1
79	Atomistic simulations of thiol-terminated modifiers for hybrid photovoltaic interfaces. Thin Solid Films, 2014, 560, 34-38.	0.8	1
80	Investigation of Siderophore-Monobactam Antibiotic Derivatives: Their Iron(III)-Complexes and Binding to Receptors. Biophysical Journal, 2017, 112, 551a-552a.	0.2	1
81	Electronic excitations of stable fullerene-like GaP clusters. Materials Research Society Symposia Proceedings, 2004, 854, U3.4.1.	0.1	0
82	Rotational profiles of molecular absorption bands in astrophysically relevant conditions: ab-initio approach. Computational Materials Science, 2004, 30, 92-97.	1.4	0
83	Modelling photoluminescence from interstellar dust. Journal of Physics: Conference Series, 2005, 6, 185-190.	0.3	0
84	Testing the attribution of selected DIBs to dehydrogenated coronene cations. Proceedings of the International Astronomical Union, 2008, 4, 67-68.	0.0	0
85	Dehydrogenated coronene cations and interstellar extinction. Proceedings of the International Astronomical Union, 2008, 4, 75-76.	0.0	0
86	Computational Study of the Interaction between Antimicrobial Compounds and Efflux Systems of Gram-Negative Bacteria. Biophysical Journal, 2017, 112, 274a.	0.2	0
87	Molecular Rationale Behind the Differential Substrate Specificity of RND Transporters AcrB and AcrD. Biophysical Journal, 2017, 112, 274a.	0.2	0
88	Transport Mechanism in the RND Transporter AcrD of E. coli. Biophysical Journal, 2017, 112, 274a.	0.2	0
89	Filtering with the Electric Field: A Story on Protein Channels Electrostatics. Biophysical Journal, 2017, 112, 417a.	0.2	0
90	Binding of Antibiotics to the Multidrug Efflux Pump AcrB of E. coli Investigated by Molecular Docking. Biophysical Journal, 2017, 112, 493a-494a.	0.2	0

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91	Bacterial Porins as Electrostatic Nanosieves: Exploring Transport Rules of Small Polar Molecules. <i>Biophysical Journal</i> , 2018, 114, 134a.	0.2	0
92	EDES: A Protocol to Generate Holo-Like and Druggable Protein Conformations Starting from the APO Structure. <i>Biophysical Journal</i> , 2020, 118, 44a.	0.2	0