GiovanniMaria Piccini

List of Publications by Year
in descending order

31	1,924	361413	434195
papers	citations	20 h-index	31 g-index

34	34	34	2114
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	Ab initio molecular dynamics with enhanced sampling in heterogeneous catalysis. Catalysis Science and Technology, 2022, 12, 12-37.	4.1	29
2	Enantioselektive Tailâ€toâ€Headâ€Terpencyclisierungen durch optisch aktive hexamere Resorcin[4]arenâ€Kapselderivate. Angewandte Chemie, 2022, 134, .	2.0	2
3	Enantioselective Tailâ€toâ€Head Terpene Cyclizations by Optically Active Hexameric Resorcin[4]arene Capsule Derivatives. Angewandte Chemie - International Edition, 2022, 61, .	13.8	17
4	Mimicry of the proton wire mechanism of enzymes inside a supramolecular capsule enables Î²-selective O-glycosylations. Nature Chemistry, 2022, 14, 985-994.	13.6	23
5	Understanding the binding properties of phosphorylated glycoluril-derived molecular tweezers and selective nanomolar binding of natural polyamines in aqueous solution. Organic and Biomolecular Chemistry, 2021, 19, 3628-3633.	2.8	3
6	Confinement effects and acid strength in zeolites. Nature Communications, 2021, 12, 2630.	12.8	90
7	Deep learning the slow modes for rare events sampling. Proceedings of the National Academy of Sciences of the United States of America, 2021, 118, .	7.1	104
8	A metadynamics perspective on the reduction mechanism of the Pt(IV) asplatin prodrug. Journal of Computational Chemistry, 2020, 41, 290-294.	3.3	3
9	Tautomeric Equilibrium in Condensed Phases. Journal of Chemical Theory and Computation, 2020, 16, 6027-6031.	5.3	6
10	Overriding Intrinsic Reactivity in Aliphatic Câ^'H Oxidation: Preferential C3/C4 Oxidation of Aliphatic Ammonium Substrates. Angewandte Chemie - International Edition, 2020, 59, 12387-12391.	13.8	16
11	Requirements for Terpene Cyclizations inside the Supramolecular Resorcinarene Capsule: Bound Water and Its Protonation Determine the Catalytic Activity. Journal of the American Chemical Society, 2020, 142, 4400-4410.	13.7	44
12	Including dispersion in density functional theory for adsorption on flat oxide surfaces, in metalâ€"organic frameworks and in acidic zeolites. Physical Chemistry Chemical Physics, 2020, 22, 7577-7585.	2.8	30
13	The reaction mechanism of the azideâ€"alkyne Huisgen cycloaddition. Physical Chemistry Chemical Physics, 2019, 21, 19281-19287.	2.8	8
14	Promoting transparency and reproducibility in enhanced molecular simulations. Nature Methods, 2019, 16, 670-673.	19.0	655
15	Accurate Quantum Chemical Free Energies at Affordable Cost. Journal of Physical Chemistry Letters, 2019, 10, 3727-3731.	4.6	20
16	Chasing the Full Free Energy Landscape of Neuroreceptor/Ligand Unbinding by Metadynamics Simulations. Journal of Chemical Theory and Computation, 2019, 15, 3354-3361.	5.3	53
17	Improving collective variables: The case of crystallization. Journal of Chemical Physics, 2019, 150, 094509.	3.0	38
18	Microscopic description of acidâ€"base equilibrium. Proceedings of the National Academy of Sciences of the United States of America, 2019, 116, 4054-4057.	7.1	28

#	Article	IF	Citations
19	Folding a small protein using harmonic linear discriminant analysis. Journal of Chemical Physics, 2018, 149, 194113.	3.0	34
20	Metadynamics with Discriminants: A Tool for Understanding Chemistry. Journal of Chemical Theory and Computation, 2018, 14, 5040-5044.	5.3	45
21	Ab initio study of methanol and ethanol adsorption on BrÃ¸nsted sites in zeolite H-MFI. Physical Chemistry Chemical Physics, 2018, 20, 19964-19970.	2.8	29
22	Collective Variables from Local Fluctuations. Journal of Physical Chemistry Letters, 2018, 9, 2776-2781.	4.6	101
23	Variational Flooding Study of a S_N2 Reaction. Journal of Physical Chemistry Letters, 2017, 8, 580-583.	4.6	23
24	Identifying Slow Molecular Motions in Complex Chemical Reactions. Journal of Physical Chemistry Letters, 2017, 8, 4197-4200.	4.6	12
25	Ab Initio Prediction of Adsorption Isotherms for Small Molecules in Metalâ€“Organic Frameworks. Journal of the American Chemical Society, 2016, 138, 14047-14056.	13.7	62
26	Abâ€…Initio Calculation of Rate Constants for Moleculeâ€“Surface Reactions with Chemical Accuracy. Angewandte Chemie, 2016, 128, 5321-5323.	2.0	13
27	Abâ€…Initio Calculation of Rate Constants for Moleculeâ€“Surface Reactions with Chemical Accuracy. Angewandte Chemie - International Edition, 2016, 55, 5235-5237.	13.8	100
28	Accurate Adsorption Thermodynamics of Small Alkanes in Zeolites. Ab initio Theory and Experiment for H-Chabazite. Journal of Physical Chemistry C, 2015, 119, 6128-6137.	3.1	120
29	Effect of Anharmonicity on Adsorption Thermodynamics. Journal of Chemical Theory and Computation, 2014, 10, 2479-2487.	5.3	101
30	Gold Nanowires: A Time-Dependent Density Functional Assessment of Plasmonic Behavior. Journal of Physical Chemistry C, 2013, 117, 17196-17204.	3.1	60
31	Quantum Chemical Free Energies: Structure Optimization and Vibrational Frequencies in Normal Modes. Journal of Chemical Theory and Computation, 2013, 9, 5038-5045.	5.3	53