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	Promoting transparency and reproducibility in enhanced molecular simulations. Nature Methods, 2019, 16, 670-673.	19.0	655
2	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
3	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
4	Effect of Anharmonicity on Adsorption Thermodynamics. Journal of Chemical Theory and Computation, 2014, 10, 2479-2487.	5.3	101
5	Collective Variables from Local Fluctuations. Journal of Physical Chemistry Letters, 2018, 9, 2776-2781.	4.6	101
6	Abâ€…Initio Calculation of Rate Constants for Moleculeâ€“Surface Reactions with Chemical Accuracy. Angewandte Chemie - International Edition, 2016, 55, 5235-5237.	13.8	100
7	Confinement effects and acid strength in zeolites. Nature Communications, 2021, 12, 2630.	12.8	90
8	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
9	Gold Nanowires: A Time-Dependent Density Functional Assessment of Plasmonic Behavior. Journal of Physical Chemistry C, 2013, 117, 17196-17204.	3.1	60
10	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
11	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
12	Metadynamics with Discriminants: A Tool for Understanding Chemistry. Journal of Chemical Theory and Computation, 2018, 14, 5040-5044.	5.3	45
13	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
14	Improving collective variables: The case of crystallization. Journal of Chemical Physics, 2019, 150, 094509.	3.0	38
15	Folding a small protein using harmonic linear discriminant analysis. Journal of Chemical Physics, 2018, 149, 194113.	3.0	34
16	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
17	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
18	Ab initio molecular dynamics with enhanced sampling in heterogeneous catalysis. Catalysis Science and Technology, 2022, 12, 12-37.	4.1	29

#	Article	IF	Citations
19	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
20	Variational Flooding Study of a S_N2 Reaction. Journal of Physical Chemistry Letters, 2017, 8, 580-583.	4.6	23
21	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
22	Accurate Quantum Chemical Free Energies at Affordable Cost. Journal of Physical Chemistry Letters, 2019, 10, 3727-3731.	4.6	20
23	Enantioselective Tailâ€toâ€Head Terpene Cyclizations by Optically Active Hexameric Resorcin[4]arene Capsule Derivatives. Angewandte Chemie - International Edition, 2022, 61, .	13.8	17
24	Overriding Intrinsic Reactivity in Aliphatic Cå^'H Oxidation: Preferential C3/C4 Oxidation of Aliphatic Ammonium Substrates. Angewandte Chemie - International Edition, 2020, 59, 12387-12391.	13.8	16
25	Abâ€...Initio Calculation of Rate Constants for Moleculeâ€“Surface Reactions with Chemical Accuracy. Angewandte Chemie, 2016, 128, 5321-5323.	2.0	13
26	Identifying Slow Molecular Motions in Complex Chemical Reactions. Journal of Physical Chemistry Letters, 2017, 8, 4197-4200.	4.6	12
27	The reaction mechanism of the azideâ€“alkyne Huisgen cycloaddition. Physical Chemistry Chemical Physics, 2019, 21, 19281-19287.	2.8	8
28	Tautomeric Equilibrium in Condensed Phases. Journal of Chemical Theory and Computation, 2020, 16, 6027-6031.	5.3	6
29	A metadynamics perspective on the reduction mechanism of the Pt(IV) asplatin prodrug. Journal of Computational Chemistry, 2020, 41, 290-294.	3.3	3
30	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
31	Enantioselektive Tailâ€toâ€Headâ€Terpencyclisierungen durch optisch aktive hexamere Resorcin[4]arenâ€Kapselderivate. Angewandte Chemie, 2022, 134, .	2.0	2