Valerie Vaissier

List of Publications by Year
in descending order

23	603	933447 10	677142 22
papers	citations	h-index	g-index

23	23	23	940
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	Exploring the role of polymer hydrophobicity in polymerâ€“metal binding thermodynamics. Physical Chemistry Chemical Physics, 2022, 24, 3579-3585.	2.8	8
2	Structural Dynamics Support Electrostatic Interactions in the Active Site of Adenylate Kinase. ChemBioChem, 2022, 23, e202200097.	2.6	4
3	Tuning the Catalytic Activity of Synthetic Enzyme KE15 with DNA. Journal of Physical Chemistry B, 2022, 126, 3407-3413.	2.6	0
4	Environment-controlled water adsorption at hydroxyapatite/collagen interfaces. Physical Chemistry Chemical Physics, 2021, 23, 13789-13796.	2.8	8
5	Critical Role of Thermal Fluctuations for CO Binding on Electrocatalytic Metal Surfaces. Jacs Au, 2021, 1, 1708-1718.	7.9	10
6	Enamel synthesis explained. Proceedings of the National Academy of Sciences of the United States of America, 2020, 117, 21847-21848.	7.1	10
7	Investigation of External Quantum Efficiency Roll-Off in OLEDs Using the Mean-Field Steady-State Kinetic Model. Journal of Physical Chemistry C, 2020, 124, 14424-14431.	3.1	2
8	ELECTRIC: Electric fields Leveraged from multipole Expansion Calculations in Tinker Rapid Interface Code. Journal of Open Source Software, 2020, 5, 2576.	4.6	9
9	Fluctuations of Electric Fields in the Active Site of the Enzyme Ketosteroid Isomerase. Journal of the American Chemical Society, 2019, 141, 12487-12492.	13.7	65
10	Computational Design of Synthetic Enzymes. Chemical Reviews, 2019, 119, 6613-6630.	47.7	133
11	Computational Optimization of Electric Fields for Improving Catalysis of a Designed Kemp Eliminase. ACS Catalysis, 2018, 8, 219-227.	11.2	70
12	Electrostatics Generated by a Supramolecular Capsule Stabilizes the Transition State for Carbonâ€“Carbon Reductive Elimination from Gold(III) Complex. Journal of Physical Chemistry Letters, 2018, 9, 3814-3818.	4.6	32
13	Geometry of Molecular Motions in Dye Monolayers at Various Coverages. Journal of Physical Chemistry C, 2017, 121, 12562-12568.	3.1	6
14	Mean field treatment of heterogeneous steady state kinetics. Chemical Physics Letters, 2017, 685, 185-190.	2.6	3
15	Quantum chemical approaches to [NiFe] hydrogenase. Essays in Biochemistry, 2017, 61, 293-303.	4.7	5
16	Evidence for photo-induced charge separation between dye molecules adsorbed to aluminium oxide surfaces. Scientific Reports, 2016, 6, 21276.	3.3	13
17	Interdye Hole Transport Accelerates Recombination in Dye Sensitized Mesoporous Films. Journal of the American Chemical Society, 2016, 138, 13197-13206.	13.7	35
18	Adiabatic Approximation in Explicit Solvent Models of RedOx Chemistry. Journal of Chemical Theory and Computation, 2016, 12, 5111-5116.	5.3	10

#	Article	IF	Citations
19	How mobile are dye adsorbates and acetonitrile molecules on the surface of TiO2 nanoparticles? A quasi-elastic neutron scattering study. Scientific Reports, 2016, 6, 39253.	3.3	6
20	Influence of Intermolecular Interactions on the Reorganization Energy of Charge Transfer between Surface-Attached Dye Molecules. Journal of Physical Chemistry C, 2015, 119, 24337-24341.	3.1	14
21	The reorganization energy of intermolecular hole hopping between dyes anchored to surfaces. Chemical Science, 2014, 5, 281-290.	7.4	60
22	Effect of Molecular Fluctuations on Hole Diffusion within Dye Monolayers. Chemistry of Materials, 2014, 26, 4731-4740.	6.7	21
23	Influence of polar medium on the reorganization energy of charge transfer between dyes in a dye sensitized film. Physical Chemistry Chemical Physics, 2013, 15, 4804.	2.8	79