

# Valerie Vaissier

## List of Publications by Year in descending order

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Version: 2024-02-01

23  
papers

603  
citations

933447

10  
h-index

677142

22  
g-index

23  
all docs

23  
docs citations

23  
times ranked

940  
citing authors

#	ARTICLE	IF	CITATIONS
1	Computational Design of Synthetic Enzymes. <i>Chemical Reviews</i> , 2019, 119, 6613-6630.	47.7	133
2	Influence of polar medium on the reorganization energy of charge transfer between dyes in a dye sensitized film. <i>Physical Chemistry Chemical Physics</i> , 2013, 15, 4804.	2.8	79
3	Computational Optimization of Electric Fields for Improving Catalysis of a Designed Kemp Eliminase. <i>ACS Catalysis</i> , 2018, 8, 219-227.	11.2	70
4	Fluctuations of Electric Fields in the Active Site of the Enzyme Ketosteroid Isomerase. <i>Journal of the American Chemical Society</i> , 2019, 141, 12487-12492.	13.7	65
5	The reorganization energy of intermolecular hole hopping between dyes anchored to surfaces. <i>Chemical Science</i> , 2014, 5, 281-290.	7.4	60
6	Interdye Hole Transport Accelerates Recombination in Dye Sensitized Mesoporous Films. <i>Journal of the American Chemical Society</i> , 2016, 138, 13197-13206.	13.7	35
7	Electrostatics Generated by a Supramolecular Capsule Stabilizes the Transition State for Carbon-Carbon Reductive Elimination from Gold(III) Complex. <i>Journal of Physical Chemistry Letters</i> , 2018, 9, 3814-3818.	4.6	32
8	Effect of Molecular Fluctuations on Hole Diffusion within Dye Monolayers. <i>Chemistry of Materials</i> , 2014, 26, 4731-4740.	6.7	21
9	Influence of Intermolecular Interactions on the Reorganization Energy of Charge Transfer between Surface-Attached Dye Molecules. <i>Journal of Physical Chemistry C</i> , 2015, 119, 24337-24341.	3.1	14
10	Evidence for photo-induced charge separation between dye molecules adsorbed to aluminium oxide surfaces. <i>Scientific Reports</i> , 2016, 6, 21276.	3.3	13
11	Adiabatic Approximation in Explicit Solvent Models of RedOx Chemistry. <i>Journal of Chemical Theory and Computation</i> , 2016, 12, 5111-5116.	5.3	10
12	Enamel synthesis explained. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2020, 117, 21847-21848.	7.1	10
13	Critical Role of Thermal Fluctuations for CO Binding on Electrocatalytic Metal Surfaces. <i>Jacs Au</i> , 2021, 1, 1708-1718.	7.9	10
14	ELECTRIC: Electric fields Leveraged from multipole Expansion Calculations in Tinker Rapid Interface Code. <i>Journal of Open Source Software</i> , 2020, 5, 2576.	4.6	9
15	Environment-controlled water adsorption at hydroxyapatite/collagen interfaces. <i>Physical Chemistry Chemical Physics</i> , 2021, 23, 13789-13796.	2.8	8
16	Exploring the role of polymer hydrophobicity in polymer-metal binding thermodynamics. <i>Physical Chemistry Chemical Physics</i> , 2022, 24, 3579-3585.	2.8	8
17	How mobile are dye adsorbates and acetonitrile molecules on the surface of TiO2 nanoparticles? A quasi-elastic neutron scattering study. <i>Scientific Reports</i> , 2016, 6, 39253.	3.3	6
18	Geometry of Molecular Motions in Dye Monolayers at Various Coverages. <i>Journal of Physical Chemistry C</i> , 2017, 121, 12562-12568.	3.1	6

#	ARTICLE	IF	CITATIONS
19	Quantum chemical approaches to [NiFe] hydrogenase. <i>Essays in Biochemistry</i> , 2017, 61, 293-303.	4.7	5
20	Structural Dynamics Support Electrostatic Interactions in the Active Site of Adenylate Kinase. <i>ChemBioChem</i> , 2022, 23, e202200097.	2.6	4
21	Mean field treatment of heterogeneous steady state kinetics. <i>Chemical Physics Letters</i> , 2017, 685, 185-190.	2.6	3
22	Investigation of External Quantum Efficiency Roll-Off in OLEDs Using the Mean-Field Steady-State Kinetic Model. <i>Journal of Physical Chemistry C</i> , 2020, 124, 14424-14431.	3.1	2
23	Tuning the Catalytic Activity of Synthetic Enzyme KE15 with DNA. <i>Journal of Physical Chemistry B</i> , 2022, 126, 3407-3413.	2.6	0