Danil S Kaliakin

List of Publications by Year
in descending order

10 papers	190 citations	1478505 6 h-index	1372567 10 g-index
10 all docs	10 docs citations	10 times ranked	261 citing authors

#	Article	IF	Citations
1	Nonadiabatic transition state theory: Application to intersystem crossings in the active sites of metalâ€sulfur proteins. International Journal of Quantum Chemistry, 2016, 116, 750-761.	2.0	71
2	3D Printed Potential and Free Energy Surfaces for Teaching Fundamental Concepts in Physical Chemistry. Journal of Chemical Education, 2015, 92, 2106-2112.	2.3	39
3	Effect of H₂ Binding on the Nonadiabatic Transition Probability between Singlet and Triplet States of the [NiFe]-Hydrogenase Active Site. Journal of Physical Chemistry A, 2015, 119, 1066-1073.	2.5	21
4	Locating Minimum Energy Crossings of Different Spin States Using the Fragment Molecular Orbital Method. Journal of Chemical Theory and Computation, 2019, 15, 6074-6084.	5.3	14
5	FMOxFMO: Elucidating Excitonic Interactions in the Fennaâ€“Matthewsâ€“Olson Complex with the Fragment Molecular Orbital Method. Journal of Chemical Theory and Computation, 2020, 16, 1175-1187.	5.3	12
6	Solution structure of a europiumâ€“nicotianamine complex supports that phytosiderophores bind lanthanides. Physical Chemistry Chemical Physics, 2021, 23, 4287-4299.	2.8	12
7	Benchmarking of Density Functionals for Z-Azoarene Half-Lives via Automated Transition State Search. Journal of Physical Chemistry A, 2021, 125, 6474-6485.	2.5	8
8	Spin-Forbidden Transitions between Electronic States in the Active Site of Rubredoxin. Journal of Physical Chemistry A, 2016, 120, 8691-8698.	2.5	7
9	The solution structures and relative stability constants of lanthanideâ€“EDTA complexes predicted from computation. Physical Chemistry Chemical Physics, 2022, 24, 10263-10271.	2.8	4
10	Spin controlled surface chemistry: alkyl desorption from Si(100)-2Ã—1 by nonadiabatic hydrogen elimination. Physical Chemistry Chemical Physics, 2020, 22, 16641-16647.	2.8	2