

# Danil S Kaliakin

## List of Publications by Year in descending order

Source: <https://exaly.com/author-pdf/6871591/publications.pdf>

Version: 2024-02-01

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