Daniela Polino

List of Publications by Year
in descending order

17	480	758635 12	887659 17
papers	citations	h-index	g-index

17	17	17	563
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	Using metadynamics to build neural network potentials for reactive events: the case of urea decomposition in water. Catalysis Today, 2022, 387, 143-149.	2.2	57
2	How Collective Phenomena Impact CO₂ Reactivity and Speciation in Different Media. Journal of Physical Chemistry A, 2020, 124, 3963-3975.	1.1	11
3	Kinetics of Aqueous Media Reactions via Ab Initio Enhanced Molecular Dynamics: The Case of Urea Decomposition. Journal of Physical Chemistry B, 2019, 123, 6851-6856.	1.2	9
4	The Onset of Dehydrogenation in Solid Ammonia Borane: An Ab Initio Metadynamics Study. Angewandte Chemie - International Edition, 2019, 58, 3976-3980.	7.2	23
5	The Onset of Dehydrogenation in Solid Ammonia Borane: An Ab Initio Metadynamics Study. Angewandte Chemie, 2019, 131, 4016-4020.	1.6	14
6	Revealing the role of phosphoric acid in all-vanadium redox flow batteries with DFT calculations and in situ analysis. Physical Chemistry Chemical Physics, 2018, 20, 23664-23673.	1.3	21
7	Identifying Slow Molecular Motions in Complex Chemical Reactions. Journal of Physical Chemistry Letters, 2017, 8, 4197-4200.	2.1	12
8	Combustion Chemistry via Metadynamics: Benzyl Decomposition Revisited. Journal of Physical Chemistry A, 2015, 119, 978-989.	1.1	18
9	On the kinetics of the C5H5+ C5H5 reaction. Proceedings of the Combustion Institute, 2013, 34, 557-564.	2.4	72
10	Predictive Theory for the Addition and Insertion Kinetics of ¹CH₂ Reacting with Unsaturated Hydrocarbons. Journal of Physical Chemistry A, 2013, 117, 12677-12692.	1.1	21
11	Analysis of Some Reaction Pathways Active during Cyclopentadiene Pyrolysis. Journal of Physical Chemistry A, 2012, 116, 3313-3324.	1.1	67
12	Is Quantum Tunneling Relevant in Freeâ€Radical Polymerization?. Macromolecular Reaction Engineering, 2012, 6, 496-506.	0.9	15
13	Toluene and benzyl decomposition mechanisms: elementary reactions and kinetic simulations. Physical Chemistry Chemical Physics, 2011, 13, 21308.	1.3	53
14	Fulvenallene Decomposition Kinetics. Journal of Physical Chemistry A, 2011, 115, 10281-10289.	1.1	42
15	Analysis of the Reactivity on the C₇H₆ Potential Energy Surface. Journal of Physical Chemistry A, 2011, 115, 7928-7936.	1.1	32
16	Theoretical investigation of germane and germylene decomposition kinetics. Physical Chemistry Chemical Physics, 2010, 12, 10622.	1.3	11
17	An Ab Initio RRKM/Master Equation Investigation of SiH4 and GeH4 Decomposition Kinetics Using a Kinetic Monte Carlo Approach. ECS Transactions, 2009, 25, 445-452.	0.3	2