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List of Publications by Year in descending order

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Version: 2024-02-01

10
papers

132
citations

1478505

6
h-index

1372567

10
g-index

13
all docs

13
docs citations

13
times ranked

229
citing authors

#	ARTICLE	IF	CITATIONS
1	(Dis)Similarities of adsorption of diverse functional groups over alumina and hematite depending on the surface state. Journal of Chemical Physics, 2021, 154, 084701.	3.0	11
2	A quantum-classical study of the effect of the long range tail of the potential on reactive and inelastic OH+H ₂ dynamics. Chemical Physics Letters, 2021, 769, 138404.	2.6	6
3	Methane Production from H ₂ + CO ₂ Reaction: An Open Molecular Science Case for Computational and Experimental Studies. Physchem, 2021, 1, 82-94.	1.1	1
4	DockOnSurf: A Python Code for the High-Throughput Screening of Flexible Molecules Adsorbed on Surfaces. Journal of Chemical Information and Modeling, 2021, 61, 3386-3396.	5.4	13
5	Density-functional tight-binding: basic concepts and applications to molecules and clusters. Advances in Physics: X, 2020, 5, 1710252.	4.1	53
6	A quantum-classical study of the OH + H ₂ reactive and inelastic collisions. Chemical Physics Letters, 2017, 674, 103-108.	2.6	8
7	Closer versus Long Range Interaction Effects on the Non-Arrhenius Behavior of Quasi-Resonant O ₂ + N ₂ Collisions. Journal of Physical Chemistry A, 2017, 121, 5088-5099.	2.5	4
8	The role of the long-range tail of the potential in O ₂ + N ₂ collisional inelastic vibrational energy transfers. Physical Chemistry Chemical Physics, 2017, 19, 11206-11211.	2.8	10
9	Methane production by CO ₂ hydrogenation reaction with and without solid phase catalysis. Fuel, 2017, 209, 802-811.	6.4	25
10	Simulation of Methane Production from Carbon Dioxide on a Collaborative Research Infrastructure. Lecture Notes in Computer Science, 2016, , 319-333.	1.3	1