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List of Publications by Year in descending order

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1478505 1372567 17 110 10 6 citations g-index h-index papers 17 17 17 152 docs citations times ranked citing authors all docs

#	Article	IF	CITATIONS
1	Theoretical study on the adsorption of carbon dioxide on individual and alkali-metal doped MOF-5s. Russian Journal of Physical Chemistry A, 2016, 90, 220-225.	0.6	19
2	Understanding the influence of single metal (Li, Mg, Al, Fe, Ag) doping on the electronic and optical properties of g-C <sub>3</sub> N <sub>4</sub> : a theoretical study. Molecular Simulation, 2021, 47, 10-17.	2.0	16
3	Theoretical study of carbon dioxide activation by metals (Co, Cu, Ni) supported on activated carbon. Journal of Molecular Modeling, 2015, 21, 322.	1.8	13
4	Ab-initio study of effect of basic MgO to V2O5 catalyst on oxidative dehydrogenation of C3H8 and n-C4H10. Applied Catalysis A: General, 2011, 407, 106-111.	4.3	8
5	Conversion of Carbon Monoxide into Methanol on Alumina-Supported Cobalt Catalyst: Role of the Support and Reaction Mechanismâ€"A Theoretical Study. Catalysts, 2019, 9, 6.	3.5	8
6	Study on the role of SBA-15 in the oxidative dehydrogenation of n-butane over vanadia catalyst using density functional theory. Journal of Molecular Modeling, 2013, 19, 3233-3243.	1.8	7
7	Study on the Adsorption and Activation Behaviours of Carbon Dioxide over Copper Cluster (Cu4) and Alumina-Supported Copper Catalyst (Cu4/Al2O3) by means of Density Functional Theory. Journal of Chemistry, 2019, 2019, 1-10.	1.9	6
8	Whether planar or corrugated graphitic carbon nitride combined with titanium dioxide exhibits better photocatalytic performance?. RSC Advances, 2021, 11, 16351-16358.	3.6	6
9	Carbon Dioxide Methanation Over Nickel Catalysts Supported on Activated Carbon at Low Temperature. Australian Journal of Chemistry, 2019, 72, 969.	0.9	5
10	A GO/CoMo <sub>3</sub> S <sub>13</sub> chalcogel heterostructure with rich catalytic Mo–S–Co bridge sites for the hydrogen evolution reaction. Nanoscale, 2022, 14, 9331-9340.	5.6	5
11	Understanding the adsorptive interactions of arsenate–iron nanoparticles with curved fullerene-like sheets in activated carbon using a quantum mechanics/molecular mechanics computational approach. Physical Chemistry Chemical Physics, 2017, 19, 14262-14268.	2.8	4
12	A Theoretical Study on the Interaction between Zinc Oxide Cluster (ZnO)3 and Mercury Ion (HgOH+). Russian Journal of Physical Chemistry A, 2020, 94, 1199-1207.	0.6	3
13	New insight into the mechanism of carbon dioxide activation on copper-based catalysts: A theoretical study. Journal of Molecular Graphics and Modelling, 2021, 107, 107979.	2.4	3
14	Physisorption and chemisorption of CO2 on Fe-MIL-88B derivatives: Impact of the functional groups on the electronic properties and adsorption tendency - A theoretical investigation. Journal of Molecular Graphics and Modelling, 2022, 112, 108124.	2.4	3
15	Effect of organic substituents on the adsorption of carbon dioxide on a metal–organic framework. Russian Journal of Physical Chemistry A, 2017, 91, 162-166.	0.6	2
16	Adsorption of lindane ( $\hat{l}^3$ -hexachlorocyclohexane) on nickel modified graphitic carbon nitride: a theoretical study. RSC Advances, 2021, 11, 21048-21056.	3.6	2
17	Integrated QMMM and Monte Carlo methods for analysis of adsorptive interactions between goethite cluster, carbon nanotubes, and arsenate. International Journal of Quantum Chemistry, 2018, 118, e25653.	2.0	О