Nguyen Ngoc Ha, Hnue

List of Publications by Year
in descending order

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

#	Article	IF	Citations
1	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
2	A GO/CoMo₃S₁₃ chalcogel heterostructure with rich catalytic Moâ€“Sâ€“Co bridge sites for the hydrogen evolution reaction. Nanoscale, 2022, 14, 9331-9340.	5.6	5
3	Whether planar or corrugated graphitic carbon nitride combined with titanium dioxide exhibits better photocatalytic performance?. RSC Advances, 2021, 11, 16351-16358.	3.6	6
4	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
5	Adsorption of lindane (Î³-hexachlorocyclohexane) on nickel modified graphitic carbon nitride: a theoretical study. RSC Advances, 2021, 11, 21048-21056.	3.6	2
6	Understanding the influence of single metal (Li, Mg, Al, Fe, Ag) doping on the electronic and optical properties of g-C₃N₄: a theoretical study. Molecular Simulation, 2021, 47, 10-17.	2.0	16
7	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
8	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
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	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
11	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	0
12	Effect of organic substituents on the adsorption of carbon dioxide on a metalâ€“organic framework. Russian Journal of Physical Chemistry A, 2017, 91, 162-166.	0.6	2
13	Understanding the adsorptive interactions of arsenateâ€“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
14	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
15	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
16	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
17	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