Mohammad Kemal Agusta

List of Publications by Year
in descending order

36	559	623734 14	677142 22
papers	citations	h-index	g-index

36	36	36	593
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	Temperature-induced orbital polarizations and tunable charge dynamics in layered double perovskite thin films. Materials Today Energy, 2022, 24, 100921.	4.7	5
2	Ethylene Carbonate Adsorption and Decomposition on Pristine and Defective ZnO(101Ì…0) Surfaces: A First-Principles Study. Journal of Physical Chemistry C, 2022, 126, 2151-2160.	3.1	5
3	Significant role of thorny surface morphology of polyaniline on adsorption of triiodide ions towards counter electrode in dye-sensitized solar cells. New Journal of Chemistry, 2021, 45, 5958-5970.	2.8	11
4	Density functional and microkinetic study of CO2 hydrogenation to methanol on subnanometer Pd cluster doped by transition metal (M= Cu, Ni, Pt, Rh). International Journal of Hydrogen Energy, 2021, 46, 14418-14428.	7.1	19
5	Distinct Behaviors of Cu- and Ni-ZSM-5 Zeolites toward the Post-activation Reactions of Methane. Journal of Physical Chemistry C, 2021, 125, 19333-19344.	3.1	6
6	Formation of Tilted FeN₄ Configuration as the Origin of Oxygen Reduction Reaction Activity Enhancement on a Pyrolyzed Fe-N-C Catalyst with FeN₄-Edge Active Sites. Journal of Physical Chemistry C, 2021, 125, 19682-19696.	3.1	12
7	Coadsorption of hydrazine and OH on the Ni(211) surface: A DFT study. Surface Science, 2021, 714, 121931.	1.9	2
8	Coadsorption of hydrazine (N2H4) and OH on NiZn surface: A DFT-based study. Surface Science, 2020, 691, 121505.	1.9	5
9	Novel Mechanistic Insights into Methane Activation over Fe and Cu Active Sites in Zeolites: A Comparative DFT Study Using Meta-GGA Functionals. Journal of Physical Chemistry C, 2020, 124, 18112-18125.	3.1	24
10	Dissociative Oxygen Reduction Reaction Mechanism on the Neighboring Active Sites of a Boron-Doped Pyrolyzed Feâ€“Nâ€“C Catalyst. Journal of Physical Chemistry C, 2020, 124, 11383-11391.	3.1	32
11	Effect of surface defects on the interaction of the oxygen molecule with the ZnO(101Ì„0) surface. New Journal of Chemistry, 2020, 44, 7376-7385.	2.8	15
12	PWDFT.jl: A Julia package for electronic structure calculation using density functional theory and plane wave basis. Computer Physics Communications, 2020, 256, 107372.	7.5	6
13	DFT and microkinetic investigation of methanol synthesis via CO₂ hydrogenation on Ni(111)-based surfaces. Physical Chemistry Chemical Physics, 2019, 21, 20276-20286.	2.8	26
14	Oxygen reduction reaction mechanism on a phosporus-doped pyrolyzed graphitic Fe/N/C catalyst. New Journal of Chemistry, 2019, 43, 11408-11418.	2.8	19
15	Density functional study of methyl butanoate adsorption and its Câ€“O bonds cleavage on MoS₂-based catalyst with various loads of Ni promoters. Journal of Physics Condensed Matter, 2019, 31, 365001.	1.8	8
16	Theoretical study of CO2 hydrogenation to methanol on isolated small Pd clusters. Journal of Energy Chemistry, 2019, 35, 79-87.	12.9	30
17	Density Functional Study on Benzene, Toluene, Ethylbenzene and Xylene Adsorptions on ZnO(100) Surface. Molekul, 2019, 14, 37.	0.3	9
18	Computational Design of Ni-Zn Based Catalyst for Direct Hydrazine Fuel Cell Catalyst Using Density Functional Theory. Procedia Engineering, 2017, 170, 148-153.	1.2	10

#	Article	IF	Citations
19	Hydrogen Adsorption on Fe-based Metal Organic Frameworks: DFT Study. Procedia Engineering, 2017, 170, 136-140.	1.2	13
20	Boron and Nitrogen Co-doping Configuration on Pyrolyzed Fe-N 4 /C Catalyst. Procedia Engineering, 2017, 170, 131-135.	1.2	14
21	Selectivity of CO and NO adsorption on ZnO (0002) surfaces: A DFT investigation. Applied Surface Science, 2017, 410, 373-382.	6.1	40
22	First principles study of oxygen molecule interaction with the graphitic active sites of a boron-doped pyrolyzed Feâ€“Nâ€“C catalyst. Physical Chemistry Chemical Physics, 2017, 19, 23497-23504.	2.8	36
23	Conformational effects on hydrazine and OH coadsorption on Ni(111): A first-principles investigation. Surface Science, 2017, 664, 185-193.	1.9	16
24	Enhanced molecular adsorption of ethylene on reduced anatase TiO₂ (001): role of surface O-vacancies. RSC Advances, 2016, 6, 92241-92251.	3.6	13
25	Computational Density Functional Theory Study of Hydrazine Adsorption on Ni(110) Surface. Advanced Materials Research, 2015, 1112, 217-220.	0.3	1
26	A Theoretical Study of Ligand Effects on the Electronic Structures of Ligated Zinc Porphyrin using Density Functional Theory. Journal of the Vacuum Society of Japan, 2014, 57, 102-110.	0.3	6
27	First Principle Study of Hydrazine and OH⁻ Co-Adsorption on Ni(111) in High Coverage System. Advanced Materials Research, 2014, 893, 35-38.	0.3	2
28	Cr, Fe - Doped Anatase TiO2 Photocatalyst: DFT+U Investigation on Band Gap. Advanced Materials Research, 2014, 893, 31-34.	0.3	3
29	Adsorption of formaldehyde and formyl intermediates on Pt, PtRu-, and PtRuMo-alloy surfaces: A density functional study. Applied Surface Science, 2013, 266, 405-409.	6.1	10
30	A First Principles Study on Zincâ€“Porphyrin Interaction with O₂in Zincâ€“Porphyrin(Oxygen) Complex. Journal of the Physical Society of Japan, 2012, 81, 124301.	1.6	17
31	Theoretical Study on Hydrazine Chemisorption on Transition Metal Surfaces. Journal of the Physical Society of Japan, 2012, 81, 124705.	1.6	11
32	First principles investigations of hydrazine adsorption conformations on Ni(111) surface. Surface Science, 2012, 606, 766-771.	1.9	45
33	First principles calculation on the adsorption of water on lithiumâ€“montmorillonite (Liâ€“MMT). Journal of Physics Condensed Matter, 2012, 24, 475506.	1.8	11
34	Theoretical study of hydrazine adsorption on Pt(111): Anti or cis?. Surface Science, 2011, 605, 1347-1353.	1.9	27
35	Hydrazine (N2H4) adsorption on Ni(100) â€“ Density functional theory investigation. Surface Science, 2010, 604, 245-251.	1.9	48
36	Pathways for SO₂dissociation on Cu(100): density functional theory. Journal of Physics Condensed Matter, 2007, 19, 365244.	1.8	2