Adhitya G Saputro

List of Publications by Year
in descending order

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48	667	567281 15	642732 23
papers	citations	h-index	g-index

48	48	48	708
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	Oxygen reduction reaction on neighboring Feâ€“N₄ and quaternary-N sites of pyrolized Fe/N/C catalyst. Physical Chemistry Chemical Physics, 2015, 17, 3059-3071.	2.8	48
2	Hollow Zinc Oxide Microsphereâ€“Multiwalled Carbon Nanotube Composites for Selective Detection of Sulfur Dioxide. ACS Applied Nano Materials, 2020, 3, 8982-8996.	5.0	42
3	Selectivity of CO and NO adsorption on ZnO (0002) surfaces: A DFT investigation. Applied Surface Science, 2017, 410, 373-382.	6.1	40
4	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
5	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
6	Theoretical study of CO2 hydrogenation to methanol on isolated small Pd clusters. Journal of Energy Chemistry, 2019, 35, 79-87.	12.9	30
7	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
8	Solvent-free, small organic lactam-assisted synthesis of ZSM-5 zeolites. Materials Letters, 2021, 290, 129501.	2.6	26
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	Comparative Study on the Catalytic Activity of the TMâ€“N₂ Active Sites (TM = Mn, Fe, Co, Ni) in the Oxygen Reduction Reaction: Density Functional Theory Study. Journal of the Physical Society of Japan, 2013, 82, 114704.	1.6	22
11	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
12	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
13	In Situ XAFS and HAXPES Analysis and Theoretical Study of Cobalt Polypyrrole Incorporated on Carbon (CoPPyC) Oxygen Reduction Reaction Catalysts for Anion-Exchange Membrane Fuel Cells. Journal of Physical Chemistry C, 2014, 118, 25480-25486.	3.1	18
14	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
15	Adsorption of O₂on Cobaltâ€“(n)Pyrrole Molecules from First-Principles Calculations. Journal of the Physical Society of Japan, 2009, 78, 094710.	1.6	16
16	Conformational effects on hydrazine and OH coadsorption on Ni(111): A first-principles investigation. Surface Science, 2017, 664, 185-193.	1.9	16
17	Tunable Concave Surface Features of Mesoporous Palladium Nanocrystals Prepared from Supramolecular Micellar Templates. ACS Applied Materials & Interfaces, 2020, 12, 51357-51365.	8.0	16
18	Oxygen Reduction Reaction on Cobaltâ€“(6)Pyrrole Cluster: Density Functional Theory Study. Journal of the Physical Society of Japan, 2012, 81, 034703.	1.6	15

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19	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
20	Two-Electron Electrochemical Reduction of CO₂ on B-Doped Niâ€“Nâ€“C Catalysts: A First-Principles Study. Journal of Physical Chemistry C, 2021, 125, 19247-19258.	3.1	15
21	Boron and Nitrogen Co-doping Configuration on Pyrolyzed Fe-N 4 /C Catalyst. Procedia Engineering, 2017, 170, 131-135.	1.2	14
22	Hydrogen Adsorption on Fe-based Metal Organic Frameworks: DFT Study. Procedia Engineering, 2017, 170, 136-140.	1.2	13
23	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
24	First principles calculation on the adsorption of water on lithiumâ€“montmorillonite (Liâ€“MMT). Journal of Physics Condensed Matter, 2012, 24, 475506.	1.8	11
25	Effect of <scp>pH</scp> on elementary steps of dopachrome conversion from firstâ€principles calculation. Pigment Cell and Melanoma Research, 2014, 27, 734-743.	3.3	10
26	Mechanism of dopachrome tautomerization into 5,6-dihydroxyindole-2-carboxylic acid catalyzed by Cu(II) based on quantum chemical calculations. Biochimica Et Biophysica Acta - General Subjects, 2015, 1850, 281-286.	2.4	10
27	Density Functional Theory Study on the Interaction of O2 and H2O2 Molecules with the Active Sites of Cobaltâ€“Polypyrrole Catalyst. Journal of the Physical Society of Japan, 2014, 83, 024707.	1.6	9
28	Enhanced NO Gas Performance of (002)-Oriented Zinc Oxide Nanostructure Thin Films. IEEE Access, 2019, 7, 155446-155454.	4.2	9
29	Density Functional Study on Benzene, Toluene, Ethylbenzene and Xylene Adsorptions on ZnO(100) Surface. Molekul, 2019, 14, 37.	0.3	9
30	Density Functional Theory Study on the Interaction of O₂ Molecule with Cobaltâ€“(6)Pyrrole Clusters. Japanese Journal of Applied Physics, 2011, 50, 055702.	1.5	8
31	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
32	Study on building machine learning model to predict biodegradable-ready materials. AIP Conference Proceedings, 2019, , .	0.4	8
33	Effects of introduction of Î±â€carboxylate, Nâ€methyl, and Nâ€formyl groups on intramolecular cyclization of oâ€quinone amines: Density functional theoryâ€based study. International Journal of Quantum Chemistry, 2017, 117, e25445.	2.0	7
34	Molecular insight into the role of zeolite lattice constraints on methane activation over the Cuâ€“Oâ€“Cu active site. Physical Chemistry Chemical Physics, 2022, 24, 4196-4203.	2.8	7
35	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
36	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

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37	Density Functional Study on the Formation of Sulfur-doped Configuration on the Active Site of Pyrolyzed Fe/N/C Catalyst. Journal of Physics: Conference Series, 2019, 1204, 012119.	0.4	5
38	Coadsorption of hydrazine (N2H4) and OH on NiZn surface: A DFT-based study. Surface Science, 2020, 691, 121505.	1.9	5
39	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
40	A Density-Functional Study on the Change of Q/B-Band Intensity Ratio of Zinc Tetraphenylporphyrin in Solvents. Journal of the Physical Society of Japan, 2014, 83, 084802.	1.6	3
41	Enhanced Lithium Diffusivity in Reduced Cerium Oxides: A First-Principles Study. Journal of Physical Chemistry C, 2022, 126, 3328-3338.	3.1	3
42	Computational Investigation on the â^™OOH Scavenging Sites of Gnetin C. Food Biophysics, 2021, 16, 337-345.	3.0	2
43	Preparation of Polycrystalline Silicon from Rice Husk by Thermal Decomposition and Aluminothermic Reduction. Molekul, 2020, 15, 26.	0.3	2
44	Frontier Orbitals of Dehydrogenated Tetrahydrocurcumin in Water Solvent: A Theoretical Study. Journal of Physics: Conference Series, 2018, 1090, 012029.	0.4	1
45	Predicting Notable Radical Scavenging Sites of Gnetin C Using Density Functional Theory. Materials Science Forum, 2019, 966, 229-233.	0.3	1
46	Effect of polyethylene glycol 6000 on the microstructure and magnetic properties of BaFe10.4Al1.6O19. Materials Research Express, 2021, 8, 036102.	1.6	1
47	Immobilization of leucine on polypyrrole for biosensor applications: A density functional theory study. , 2009, , .		0
48	Theoretical study on frontier orbitals of dehydrogenated tetrahydrocurcumin in gas phase. Journal of Physics: Conference Series, 2019, 1204, 012019.	0.4	0