Baojun Wang

List of Publications by Year
in descending order

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30	781	471509 17	501196 28
papers	citations	h-index	g-index

30	30	30	831
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	The active site of ethanol formation from syngas over Cu4 cluster modified MoS2 catalyst: A theoretical investigation. Applied Surface Science, 2021, 540, 148301.	6.1	4
2	C2H2 semi-hydrogenation over the supported Pd and Cu catalysts: The effects of the support types, properties and metal-support interaction on C2H4 selectivity and activity. Applied Surface Science, 2020, 503, 144142.	6.1	15
3	Syngas-to-C2 oxygenates on Cu-based catalyst: Quantitative insight into the balancing effect of active Cuî+(0Ââ‰ÂîÂâ‰Â1) sites. Chemical Engineering Science, 2020, 224, 115785.	3.8	10
4	Crystal facet dependence of carbon chain growth mechanism over the Hcp and Fcc Co catalysts in the Fischer-Tropsch synthesis. Applied Catalysis B: Environmental, 2020, 269, 118847.	20.2	29
5	The new role of surface adsorbed CH (xâ€¯=â€¯1â€“3) intermediates as a co-adsorbed promoter in self-promoting syngas conversion to form CH intermediates and C2 oxygenates on the Rh-doped Cu catalyst. Journal of Catalysis, 2019, 377, 1-12.	6.2	18
6	PdIn intermetallic material with isolated single-atom Pd sites â€“ A promising catalyst for direct formic acid fuel cell. Chemical Engineering Science, 2019, 199, 64-78.	3.8	25
7	DFT study on CO oxidative coupling to DMO over Pd4/TiO2 and Pd4/TiO2-Ov: A role of oxygen vacancy on support. Computational Materials Science, 2019, 159, 1-11.	3.0	11
8	Insight into the C C chain growth in Fischer-Tropsch synthesis on HCP Co(10-10) surface: The effect of crystal facets on the preferred mechanism. Computational Materials Science, 2018, 145, 263-279.	3.0	16
9	Density functional theory calculations and analysis for the reduction of NO by H2 on Pd6/TiO2. Computational Materials Science, 2018, 149, 182-190.	3.0	8
10	Insight into the role of the promoters Pt, Ru and B in inhibiting the deactivation of Co catalysts in Fischer-Tropsch synthesis. Applied Surface Science, 2018, 453, 309-319.	6.1	16
11	Insight into size dependence of C 2 oxygenate synthesis from syngas on Cu cluster: The effect of cluster size on the selectivity. Applied Surface Science, 2017, 407, 282-296.	6.1	22
12	Catalytic selectivity of Rh/TiO₂catalyst in syngas conversion to ethanol: probing into the mechanism and functions of TiO₂support and promoter. Catalysis Science and Technology, 2017, 7, 1073-1085.	4.1	31
13	Insight into the influence of addition of a second metal Fe and supports with different morphology on H 2 dissociation over Ni/MgO catalysts. Applied Surface Science, 2017, 426, 827-832.	6.1	1
14	Insight into the preferred formation mechanism of long-chain hydrocarbons in Fischerâ€“Tropsch synthesis on Hcp Co(10â¯11) surfaces from DFT and microkinetic modeling. Catalysis Science and Technology, 2017, 7, 3758-3776.	4.1	39
15	Formation of C₂oxygenates and ethanol from syngas on an Fe-decorated Cu-based catalyst: insight into the role of Fe as a promoter. Physical Chemistry Chemical Physics, 2017, 19, 30883-30894.	2.8	21
16	Unraveling the role of support surface hydroxyls and its effect on the selectivity of C2 species over Rh/Î³-Al2O3 catalyst in syngas conversion: A theoretical study. Applied Surface Science, 2016, 379, 384-394.	6.1	13
17	Insight into CH x formation in Fischerâ€“Tropsch synthesis on the hexahedron Co catalyst: Effect of surface structure on the preferential mechanism and existence form. Applied Catalysis A: General, 2016, 525, 76-84.	4.3	18
18	Insight into the mechanism about the initiation, growth and termination of the Câ€“C chain in syngas conversion on the Co(0001) surface: a theoretical study. Physical Chemistry Chemical Physics, 2016, 18, 27272-27283.	2.8	30

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19	First-Principles Study about the Effect of Coverage on H₂ Adsorption and Dissociation over a Rh(100) Surface. Journal of Physical Chemistry C, 2015, 119, 10355-10364.	3.1	17
20	CH4 dehydrogenation on Cu(111), Cu@Cu(111), Rh@Cu(111) and RhCu(111) surfaces: A comparison studies of catalytic activity. Applied Surface Science, 2015, 341, 100-108.	6.1	30
21	Source and major species of CH_x (x = 1â€“3) in acetic acid synthesis from methaneâ€“syngas on Rh catalyst: a theoretical study. RSC Advances, 2014, 4, 58631-58642.	3.6	5
22	Ethanol Synthesis from Syngas on the Stepped Rh(211) Surface: Effect of Surface Structure and Composition. Journal of Physical Chemistry C, 2014, 118, 22691-22701.	3.1	46
23	The adsorption and dissociation of methane on cobalt surfaces: thermochemistry and reaction barriers. RSC Advances, 2014, 4, 43004-43011.	3.6	25
24	Fundamental studies about the interaction of water with perfect, oxygen-vacancy and pre-covered oxygen Cu2O(1 1 1) surfaces: Thermochemistry, barrier, product. Applied Surface Science, 2013, 279, 260-271.	6.1	31
25	Insights into the preference of CHx(x=1â€“3) formation from CO hydrogenation on Cu(111) surface. Applied Surface Science, 2013, 265, 720-730.	6.1	51
26	Insight into the preference mechanism for CC chain formation of C2 oxygenates and the effect of promoters in syngas conversion over Cu-based catalysts. Applied Catalysis A: General, 2013, 466, 77-89.	4.3	25
27	Insights into the mechanism of ethanol formation from syngas on Cu and an expanded prediction of improved Cu-based catalyst. Journal of Catalysis, 2013, 305, 238-255.	6.2	129
28	Insights into the effect of surface hydroxyls on CO2 hydrogenation over Pd/Î³-Al2O3 catalyst: A computational study. Applied Catalysis B: Environmental, 2012, 126, 108-120.	20.2	62
29	The role of CS2 in CS2/NMP mixed solvent in weakening the hydrogen bond of OHâ€“N in coal: a DFT investigation. Journal of Molecular Modeling, 2012, 18, 921-927.	1.8	2
30	Solvent effects on Cu2O(111) surface properties and CO adsorption on Cu2O(111) surface: A DFT study. Applied Catalysis A: General, 2011, 400, 142-147.	4.3	31