

Baojun Wang

List of Publications by Year in descending order

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30
papers

781
citations

471509
17
h-index

501196
28
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30
all docs

30
docs citations

30
times ranked

831
citing authors

#	ARTICLE	IF	CITATIONS
1	Insights into the mechanism of ethanol formation from syngas on Cu and an expanded prediction of improved Cu-based catalyst. <i>Journal of Catalysis</i> , 2013, 305, 238-255.	6.2	129
2	Insights into the effect of surface hydroxyls on CO ₂ hydrogenation over Pd/γ-Al ₂ O ₃ catalyst: A computational study. <i>Applied Catalysis B: Environmental</i> , 2012, 126, 108-120.	20.2	62
3	Insights into the preference of CH _x (x=1~3) formation from CO hydrogenation on Cu(111) surface. <i>Applied Surface Science</i> , 2013, 265, 720-730.	6.1	51
4	Ethanol Synthesis from Syngas on the Stepped Rh(211) Surface: Effect of Surface Structure and Composition. <i>Journal of Physical Chemistry C</i> , 2014, 118, 22691-22701.	3.1	46
5	Insight into the preferred formation mechanism of long-chain hydrocarbons in Fischer-Tropsch synthesis on Hcp Co(10~11) surfaces from DFT and microkinetic modeling. <i>Catalysis Science and Technology</i> , 2017, 7, 3758-3776.	4.1	39
6	Solvent effects on Cu ₂ O(111) surface properties and CO adsorption on Cu ₂ O(111) surface: A DFT study. <i>Applied Catalysis A: General</i> , 2011, 400, 142-147.	4.3	31
7	Fundamental studies about the interaction of water with perfect, oxygen-vacancy and pre-covered oxygen Cu ₂ O(1 1 1) surfaces: Thermochemistry, barrier, product. <i>Applied Surface Science</i> , 2013, 279, 260-271.	6.1	31
8	Catalytic selectivity of Rh/TiO ₂ catalyst in syngas conversion to ethanol: probing into the mechanism and functions of TiO ₂ support and promoter. <i>Catalysis Science and Technology</i> , 2017, 7, 1073-1085.	4.1	31
9	CH ₄ dehydrogenation on Cu(111), Cu@Cu(111), Rh@Cu(111) and RhCu(111) surfaces: A comparison studies of catalytic activity. <i>Applied Surface Science</i> , 2015, 341, 100-108.	6.1	30
10	Insight into the mechanism about the initiation, growth and termination of the C chain in syngas conversion on the Co(0001) surface: a theoretical study. <i>Physical Chemistry Chemical Physics</i> , 2016, 18, 27272-27283.	2.8	30
11	Crystal facet dependence of carbon chain growth mechanism over the Hcp and Fcc Co catalysts in the Fischer-Tropsch synthesis. <i>Applied Catalysis B: Environmental</i> , 2020, 269, 118847.	20.2	29
12	Insight into the preference mechanism for CC chain formation of C ₂ oxygenates and the effect of promoters in syngas conversion over Cu-based catalysts. <i>Applied Catalysis A: General</i> , 2013, 466, 77-89.	4.3	25
13	The adsorption and dissociation of methane on cobalt surfaces: thermochemistry and reaction barriers. <i>RSC Advances</i> , 2014, 4, 43004-43011.	3.6	25
14	PdIn intermetallic material with isolated single-atom Pd sites – A promising catalyst for direct formic acid fuel cell. <i>Chemical Engineering Science</i> , 2019, 199, 64-78.	3.8	25
15	Insight into size dependence of C ₂ oxygenate synthesis from syngas on Cu cluster: The effect of cluster size on the selectivity. <i>Applied Surface Science</i> , 2017, 407, 282-296.	6.1	22
16	Formation of C ₂ oxygenates and ethanol from syngas on an Fe-decorated Cu-based catalyst: insight into the role of Fe as a promoter. <i>Physical Chemistry Chemical Physics</i> , 2017, 19, 30883-30894.	2.8	21
17	Insight into CH _x formation in Fischer-Tropsch synthesis on the hexahedron Co catalyst: Effect of surface structure on the preferential mechanism and existence form. <i>Applied Catalysis A: General</i> , 2016, 525, 76-84.	4.3	18
18	The new role of surface adsorbed CH (x=1~3) intermediates as a co-adsorbed promoter in self-promoting syngas conversion to form CH intermediates and C ₂ oxygenates on the Rh-doped Cu catalyst. <i>Journal of Catalysis</i> , 2019, 377, 1-12.	6.2	18

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19	First-Principles Study about the Effect of Coverage on H ₂ Adsorption and Dissociation over a Rh(100) Surface. Journal of Physical Chemistry C, 2015, 119, 10355-10364.	3.1	17
20	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
21	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
22	C ₂ H ₂ semi-hydrogenation over the supported Pd and Cu catalysts: The effects of the support types, properties and metal-support interaction on C ₂ H ₄ selectivity and activity. Applied Surface Science, 2020, 503, 144142.	6.1	15
23	Unraveling the role of support surface hydroxyls and its effect on the selectivity of C ₂ species over Rh/I ³ -Al ₂ O ₃ catalyst in syngas conversion: A theoretical study. Applied Surface Science, 2016, 379, 384-394.	6.1	13
24	DFT study on CO oxidative coupling to DMO over Pd ₄ /TiO ₂ and Pd ₄ /TiO ₂ -Ov: A role of oxygen vacancy on support. Computational Materials Science, 2019, 159, 1-11.	3.0	11
25	Syngas-to-C ₂ oxygenates on Cu-based catalyst: Quantitative insight into the balancing effect of active Cu ⁺ /(O ²⁻) sites. Chemical Engineering Science, 2020, 224, 115785.	3.8	10
26	Density functional theory calculations and analysis for the reduction of NO by H ₂ on Pd ₆ /TiO ₂ . Computational Materials Science, 2018, 149, 182-190.	3.0	8
27	Source and major species of CH _x (x = 1-3) in acetic acid synthesis from methane "syngas" on Rh catalyst: a theoretical study. RSC Advances, 2014, 4, 58631-58642.	3.6	5
28	The active site of ethanol formation from syngas over Cu ₄ cluster modified MoS ₂ catalyst: A theoretical investigation. Applied Surface Science, 2021, 540, 148301.	6.1	4
29	The role of CS ₂ in CS ₂ /NMP mixed solvent in weakening the hydrogen bond of OH-N in coal: a DFT investigation. Journal of Molecular Modeling, 2012, 18, 921-927.	1.8	2
30	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