

Xiangjian Shen

List of Publications by Year in descending order

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32
papers

1,169
citations

623574

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395590

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docs citations

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times ranked

1071
citing authors

#	ARTICLE	IF	CITATIONS
1	NiCoP nanowire@NiCo-layered double hydroxides nanosheet heterostructure for flexible asymmetric supercapacitors. <i>Chemical Engineering Journal</i> , 2020, 384, 123373.	6.6	219
2	Electronic Structure Engineering of Single-Atom Ru Sites via Co ²⁺ N ₄ Sites for Bifunctional pH-Universal Water Splitting. <i>Advanced Materials</i> , 2022, 34, e2110103.	11.1	199
3	In Situ Reconstruction of V ³⁺ -Doped Ni ₂ P Precatalysts with Tunable Electronic Structures for Water Oxidation. <i>Advanced Functional Materials</i> , 2021, 31, 2100614.	7.8	129
4	Engineering the Activity and Stability of MOF-Nanocomposites for Efficient Water Oxidation. <i>Advanced Energy Materials</i> , 2021, 11, 2003759.	10.2	108
5	The origin of palladium particle size effects in the direct synthesis of H ₂ O ₂ : Is smaller better?. <i>Journal of Catalysis</i> , 2017, 349, 30-40.	3.1	98
6	Methane dissociation on Ni(111): A fifteen-dimensional potential energy surface using neural network method. <i>Journal of Chemical Physics</i> , 2015, 143, 144701.	1.2	68
7	CH ₄ dissociation on Ni(111): a quantum dynamics study of lattice thermal motion. <i>Physical Chemistry Chemical Physics</i> , 2015, 17, 25499-25504.	1.3	41
8	Construction of graphene oxide based mixed matrix membranes with CO ₂ -philic sieving gas-transport channels through strong π - π interactions. <i>Journal of Materials Chemistry A</i> , 2018, 6, 17854-17860.	5.2	35
9	Tuning the surface energy density of non-stoichiometric LaCoO ₃ perovskite for enhanced water oxidation. <i>Journal of Power Sources</i> , 2020, 478, 228748.	4.0	33
10	Communication: Methane dissociation on Ni(111) surface: Importance of azimuth and surface impact site. <i>Journal of Chemical Physics</i> , 2016, 144, 101101.	1.2	30
11	Hydrogen diffusion on Fe surface and into subsurface from first principles. <i>Surface Science</i> , 2016, 654, 48-55.	0.8	21
12	Hydrogen diffusion into the subsurfaces of model metal catalysts from first principles. <i>Physical Chemistry Chemical Physics</i> , 2017, 19, 3557-3564.	1.3	21
13	Water dissociating on rigid Ni(100): A quantum dynamics study on a full-dimensional potential energy surface. <i>Journal of Chemical Physics</i> , 2018, 148, 144705.	1.2	20
14	Diffusion mechanisms of metal atoms in Pd Au bimetallic catalyst under CO atmosphere based on ab initio molecular dynamics. <i>Applied Surface Science</i> , 2019, 483, 991-1005.	3.1	19
15	Eight-Dimensional Quantum Dynamics Study of CH ₄ and CD ₄ Dissociation on Ni(100) Surface. <i>Journal of Physical Chemistry C</i> , 2016, 120, 20199-20205.	1.5	12
16	Dissociative chemisorption of O ₂ on Ag _n and Ag _n Ir (n = 3-26) clusters: a first-principle study. <i>Physical Chemistry Chemical Physics</i> , 2020, 22, 9053-9066.	1.3	11
17	A Synergistic effect on the atomic cluster M ₄ supported on MN ₄ -graphene (M) Tj ETQq1 1 0.784314 rgBT /Ov 11704-11712.	1.3	11
18	Abnormal subsurface hydrogen diffusion behaviors in heterogeneous hydrogenation reactions. <i>Journal of Chemical Physics</i> , 2018, 149, 174704.	1.2	10

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19	Methane activation on single-atom Ir-doped metal nanoparticles from first principles. <i>Physical Chemistry Chemical Physics</i> , 2021, 23, 15564-15573.	1.3	10
20	Hot-Atom Mechanism in Syngas Methanation on Precovered Pd(100) Surfaces. <i>Journal of Physical Chemistry Letters</i> , 2020, 11, 5312-5317.	2.1	9
21	Methane dissociation on Ni(111): A seven-dimensional to nine-dimensional quantum dynamics study. <i>Journal of Chemical Physics</i> , 2017, 147, 024702.	1.2	8
22	Enhanced diffusion and permeation of hydrogen species on the partially carbon covered iron surfaces. <i>Applied Surface Science</i> , 2020, 515, 145899.	3.1	8
23	Curvature Effects on the Magnetism of Ultrashort Zigzag Carbon Nanotubes and Nanographenes. <i>Journal of Physical Chemistry C</i> , 2010, 114, 7553-7557.	1.5	7
24	Hydrogen evolution reaction on transition metal nanoparticles from first-principles. <i>Applied Surface Science</i> , 2021, 570, 151211.	3.1	7
25	A simulated-TPD study of H ₂ desorption on metal surfaces. <i>Surface Science</i> , 2022, 718, 122015.	0.8	7
26	A thermodynamics study of hydrogen interaction with (1 1 0) transition metal surfaces. <i>Applied Surface Science</i> , 2021, 545, 148961.	3.1	6
27	Improved oxidation of hydrogen off-gas by hydrophobic surface modification: A multiscale density functional theory study. <i>Particuology</i> , 2019, 44, 28-35.	2.0	4
28	High chemisorption abilities of hydrogen and oxygen on ultrasmall iron clusters: A first-principles study. <i>Chemical Physics Letters</i> , 2018, 705, 59-64.	1.2	3
29	Oxygen Evolution Reaction: Engineering the Activity and Stability of MOF@Nanocomposites for Efficient Water Oxidation (<i>Adv. Energy Mater.</i> 16/2021). <i>Advanced Energy Materials</i> , 2021, 11, 2170063.	10.2	3
30	Theoretical new insights into hydrogen interaction with single-atom Zn- and co-doped copper metal catalysts. <i>Applied Surface Science</i> , 2021, 551, 149365.	3.1	2
31	Enhanced effect of H ₂ O monolayer on metal doped nitrogen-containing graphene for hydrogen evolution reactions. <i>Chemical Engineering Journal</i> , 2022, 431, 133283.	6.6	2
32	Hydrogen diffusion on and into the hydrogen-covered Pd(1 0 0) surfaces from first-principles. <i>Chemical Physics Letters</i> , 2022, 794, 139509.	1.2	2