Xiangjian Shen

List of Publications by Year
in descending order

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32 papers	1,169 citations	623734 14 h-index	395702 33 g-index
33 all docs	33 docs citations	33 times ranked	1071 citing authors

#	Article	IF	Citations
1	NiCoP nanowire@NiCo-layered double hydroxides nanosheet heterostructure for flexible asymmetric supercapacitors. Chemical Engineering Journal, 2020, 384, 123373.	12.7	219
2	Electronic Structure Engineering of Singleâ€Atom Ru Sites via Coâ€“N4 Sites for Bifunctional pHâ€Universal Water Splitting. Advanced Materials, 2022, 34, e2110103.	21.0	199
3	In Situ Reconstruction of Vâ€Doped Ni₂P Preâ€Catalysts with Tunable Electronic Structures for Water Oxidation. Advanced Functional Materials, 2021, 31, 2100614.	14.9	129
4	Engineering the Activity and Stability of MOFâ€Nanocomposites for Efficient Water Oxidation. Advanced Energy Materials, 2021, 11, 2003759.	19.5	108
5	The origin of palladium particle size effects in the direct synthesis of H2O2: Is smaller better?. Journal of Catalysis, 2017, 349, 30-40.	6.2	98
6	Methane dissociation on Ni(111): A fifteen-dimensional potential energy surface using neural network method. Journal of Chemical Physics, 2015, 143, 144701.	3.0	68
7	CH₄ dissociation on Ni(111): a quantum dynamics study of lattice thermal motion. Physical Chemistry Chemical Physics, 2015, 17, 25499-25504.	2.8	41
8	Construction of graphene oxide based mixed matrix membranes with CO₂-philic sieving gas-transport channels through strong Ï€â€“Ï€ interactions. Journal of Materials Chemistry A, 2018, 6, 17854-17860.	10.3	35
9	Tuning the surface energy density of non-stoichiometric LaCoO3 perovskite for enhanced water oxidation. Journal of Power Sources, 2020, 478, 228748.	7.8	33
10	Communication: Methane dissociation on Ni(111) surface: Importance of azimuth and surface impact site. Journal of Chemical Physics, 2016, 144, 101101.	3.0	30
11	Hydrogen diffusion on Fe surface and into subsurface from first principles. Surface Science, 2016, 654, 48-55.	1.9	21
12	Hydrogen diffusion into the subsurfaces of model metal catalysts from first principles. Physical Chemistry Chemical Physics, 2017, 19, 3557-3564.	2.8	21
13	Water dissociating on rigid Ni(100): A quantum dynamics study on a full-dimensional potential energy surface. Journal of Chemical Physics, 2018, 148, 144705.	3.0	20
14	Diffusion mechanisms of metal atoms in Pd Au bimetallic catalyst under CO atmosphere based on ab initio molecular dynamics. Applied Surface Science, 2019, 483, 991-1005.	6.1	19
15	Eight-Dimensional Quantum Dynamics Study of CH₄ and CD₄ Dissociation on Ni(100) Surface. Journal of Physical Chemistry C, 2016, 120, 20199-20205.	3.1	12
16	Dissociative chemisorption of O2 on Agn and Agnâ^'1Ir (n = 3â€“26) clusters: a first-principle study. Physical Chemistry Chemical Physics, 2020, 22, 9053-9066.	2.8	11
17	A Synergistic effect on the atomic cluster M₄ supported on MN₄-graphene (M) Tj ETQq1 1 0.784314 rgBT /O 11704-11712.	2.8	11
18	Abnormal subsurface hydrogen diffusion behaviors in heterogeneous hydrogenation reactions. Journal of Chemical Physics, 2018, 149, 174704.	3.0	10

#	Article	IF	Citations
19	Methane activation on single-atom Ir-doped metal nanoparticles from first principles. Physical Chemistry Chemical Physics, 2021, 23, 15564-15573.	2.8	10
20	Hot-Atom Mechanism in Syngas Methanation on Precovered Pd(100) Surfaces. Journal of Physical Chemistry Letters, 2020, 11, 5312-5317.	4.6	9
21	Methane dissociation on Ni(111): A seven-dimensional to nine-dimensional quantum dynamics study. Journal of Chemical Physics, 2017, 147, 024702.	3.0	8
22	Enhanced diffusion and permeation of hydrogen species on the partially carbon covered iron surfaces. Applied Surface Science, 2020, 515, 145899.	6.1	8
23	Curvature Effects on the Magnetism of Ultrashort Zigzag Carbon Nanotubes and Nanographenes. Journal of Physical Chemistry C, 2010, 114, 7553-7557.	3.1	7
24	Hydrogen evolution reaction on transition metal nanoparticles from first-principles. Applied Surface Science, 2021, 570, 151211.	6.1	7
25	A simulated-TPD study of H2 desorption on metal surfaces. Surface Science, 2022, 718, 122015.	1.9	7
26	A thermodynamics study of hydrogen interaction with (1 1 0) transition metal surfaces. Applied Surface Science, 2021, 545, 148961.	6.1	6
27	Improved oxidation of hydrogen off-gas by hydrophobic surface modification: A multiscale density functional theory study. Particuology, 2019, 44, 28-35.	3.6	4
28	High chemisorption abilities of hydrogen and oxygen on ultrasmall iron clusters: A first-principles study. Chemical Physics Letters, 2018, 705, 59-64.	2.6	3
29	Oxygen Evolution Reaction: Engineering the Activity and Stability of MOFâ€Nanocomposites for Efficient Water Oxidation (Adv. Energy Mater. 16/2021). Advanced Energy Materials, 2021, 11, 2170063.	19.5	3
30	Theoretical new insights into hydrogen interaction with single-atom Zn- and co-doped copper metal catalysts. Applied Surface Science, 2021, 551, 149365.	6.1	2
31	Enhanced effect of H2O monolayer on metal doped nitrogen-containing graphene for hydrogen evolution reactions. Chemical Engineering Journal, 2022, 431, 133283.	12.7	2
32	Hydrogen diffusion on and into the hydrogen-covered Pd(1 0 0) surfaces from first-principles. Chemical Physics Letters, 2022, 794, 139509.	2.6	2