Duy Le

List of Publications by Year in descending order

Source: https://exaly.com/author-pdf/665871/publications.pdf

Version: 2024-02-01

64	2,267	331259	214527
papers	citations	21 h-index	47 g-index

67	67	67	4509
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	Methanol carbonylation to acetaldehyde on Au particles supported by single-layer MoS₂ grown on silica. Journal of Physics Condensed Matter, 2022, 34, 104005.	0.7	1
2	Ligand-coordination effects on the selective hydrogenation of acetylene in single-site Pd-ligand supported catalysts. Journal of Catalysis, 2022, 413, 81-92.	3.1	8
3	Syngas molecules as probes for defects in 2D hexagonal boron nitride: their adsorption and vibrations. Physical Chemistry Chemical Physics, 2021, 23, 7988-8001.	1.3	9
4	Mechanically Enhanced Catalytic Reduction of Carbon Dioxide over Defect Hexagonal Boron Nitride. ACS Sustainable Chemistry and Engineering, 2021, 9, 2447-2455.	3.2	25
5	Fermi surfaces of the topological semimetal CaSn₃ probed through de Haas van Alphen oscillations. Journal of Physics Condensed Matter, 2021, 33, 17LT01.	0.7	4
6	Toward alcohol synthesis from CO hydrogenation on Cu(111)-supported MoS2 â€“ predictions from DFT+KMC. Journal of Chemical Physics, 2021, 154, 174701.	1.2	3
7	Modeling carrier mobility in graphene as a sensitive probe of molecular magnets. Physical Review B, 2021, 103, .	1.1	1
8	On stabilizing spin crossover molecule [Fe(tBu₂qsal)₂] on suitable supports: insights from ab initio studies. Journal of Physics Condensed Matter, 2021, 33, 385201.	0.7	1
9	Anisotropic Properties of Quasiâ€1D In₄Se₃: Mechanical Exfoliation, Electronic Transport, and Polarizationâ€Dependent Photoresponse. Advanced Functional Materials, 2021, 31, 2106459.	7.8	11
10	Asymmetric Design of Spin-Crossover Complexes to Increase the Volatility for Surface Deposition. Journal of the American Chemical Society, 2021, 143, 14563-14572.	6.6	16
11	Growth of Graphene Nanoflakes/hâ€BN Heterostructures. Advanced Materials Interfaces, 2021, 8, 2100766.	1.9	5
12	Tailoring the redox capabilities of organic ligands for metal-ligand coordination with vanadium single-sites. Surface Science, 2021, 712, 121888.	0.8	1
13	Characteristics of Single-Molecule Magnet Dimers ([Mn₃]₂) on Graphene and h-BN. Journal of Physical Chemistry C, 2020, 124, 28186-28200.	1.5	11
14	MoS2-supported Au31 for CO hydrogenation: A first-principle study. Journal of Vacuum Science and Technology A: Vacuum, Surfaces and Films, 2020, 38, 032201.	0.9	0
15	Catalytic C2H2 synthesis via low temperature CO hydrogenation on defect-rich 2D-MoS2 and 2D-MoS2 decorated with Mo clusters. Journal of Chemical Physics, 2020, 152, 074706.	1.2	3
16	Metallicity of 2H-MoS₂ induced by Au hybridization. 2D Materials, 2020, 7, 025021.	2.0	17
17	CO Oxidation Mechanisms on CoO_x-Pt Thin Films. Journal of the American Chemical Society, 2020, 142, 8312-8322.	6.6	39
18	Self-Catalyzed, Low-Temperature Atomic Layer Deposition of Ruthenium Metal Using Zero-Valent Ru(DMBD)(CO)₃ and Water. Chemistry of Materials, 2019, 31, 1304-1317.	3.2	20

#	Article	IF	Citations
19	Analysis of the fluorescence of mechanically processed defect-laden hexagonal boron nitride and the role of oxygen in catalyst deactivation. Advances in Applied Ceramics, 2019, 118, 153-158.	0.6	5
20	MoS₂ Nanoclusters Grown on TiO₂: Evidence for New Adsorption Sites at Edges and Sulfur Vacancies. Journal of Physical Chemistry C, 2019, 123, 7185-7201.	1.5	18
21	Multiâ€electron Reduction Capacity and Multiple Binding Pockets in Metalâ€“Organic Redox Assembly at Surfaces. Chemistry - A European Journal, 2019, 25, 5565-5573.	1.7	7
22	A Single Layer of MoS2 Activates Gold for Room Temperature CO Oxidation on an Inert Silica Substrate. Journal of Physical Chemistry C, 2019, 123, 6592-6598.	1.5	11
23	Methoxy Formation Induced Defects on MoS₂. Journal of Physical Chemistry C, 2018, 122, 10042-10049.	1.5	11
24	Redox-active ligand controlled selectivity of vanadium oxidation on Au(100). Chemical Science, 2018, 9, 1674-1685.	3.7	24
25	High Catalytic Activity of Pd₁/ZnO(101Ì…0) toward Methanol Partial Oxidation: A DFT+KMC Study. ACS Catalysis, 2018, 8, 5553-5569.	5.5	26
26	Gold Dispersion and Activation on the Basal Plane of Single-Layer MoS₂. Journal of Physical Chemistry C, 2018, 122, 267-273.	1.5	16
27	Redox Isomeric Surface Structures Are Preferred over Oddâ€Electron Pt 1+. Chemistry - A European Journal, 2018, 24, 15852-15858.	1.7	7
28	Two-Dimensional Folding of Polypeptides into Molecular Nanostructures at Surfaces. ACS Nano, 2017, 11, 2420-2427.	7.3	35
29	Effect of Single-Layer MoS₂ on the Geometry, Electronic Structure, and Reactivity of Transition Metal Nanoparticles. Journal of Physical Chemistry C, 2017, 121, 7282-7293.	1.5	20
30	Adsorbate doping of MoS₂and WSe₂: the influence of Na and Co. Journal of Physics Condensed Matter, 2017, 29, 285501.	0.7	12
31	MoS₂-supported gold nanoparticle for CO hydrogenation. Journal of Physics Condensed Matter, 2017, 29, 415201.	0.7	12
32	Structural Stability of N-Alkyl-Functionalized Titanium Metalâ€“Organic Frameworks in Aqueous and Humid Environments. ACS Applied Materials & Interfaces, 2017, 9, 44529-44533.	4.0	33
33	CO adsorption on Pd(111) at 0.5ML: A first principles study. Surface Science, 2017, 655, 7-11.	0.8	12
34	Ptâ€“dipyridyl tetrazine metalâ€“organic network on the Au(100) surface: insights from first principles calculations. Faraday Discussions, 2017, 204, 83-95.	1.6	4
35	Heterogeneous Metal-Free Hydrogenation over Defect-Laden Hexagonal Boron Nitride. ACS Omega, 2016, 1, 1343-1354.	1.6	43
36	Band structure characterization of WS2 grown by chemical vapor deposition. Applied Physics Letters, 2016, 108, .	1.5	40

#	Article	IF	Citations
37	The symmetry-resolved electronic structure of 2H-WSe₂(0â€‰0â€‰0â€‰1). Journal of Physics Condensed Matter, 2016, 28, 345503.	0.7	7
38	Disorder effect on the anisotropic resistivity of phosphorene determined by a tight-binding model. Physical Review B, 2016, 94, .	1.1	20
39	pH-Induced Surface Modification of Atomically Precise Silver Nanoclusters: An Approach for Tunable Optical and Electronic Properties. Inorganic Chemistry, 2016, 55, 11522-11528.	1.9	10
40	Scattering strength of the scatterer inducing variability in graphene on silicon oxide. Journal of Physics Condensed Matter, 2016, 28, 115301.	0.7	3
41	Spinâ€“orbit coupling in the band structure of monolayer WSe₂. Journal of Physics Condensed Matter, 2015, 27, 182201.	0.7	67
42	Effect of monolayer supports on the electronic structure of single-layer MoS2. IOP Conference Series: Materials Science and Engineering, 2015, 76, 012011.	0.3	8
43	Symmetry-resolved surface-derived electronic structure of MoS₂(0â€‰0â€‰0â€‰1). Journal of Physics Condensed Matter, 2014, 26, 455501.	0.7	9
44	Occupied and unoccupied electronic structure of Na doped MoS2(0001). Applied Physics Letters, 2014, 105, .	1.5	30
45	2â€Dimensional Transition Metal Dichalcogenides with Tunable Direct Band Gaps: MoS_{2(1â€“x)}Se_{2x} Monolayers. Advanced Materials, 2014, 26, 1399-1404.	11.1	334
46	Single-Layer MoS₂ with Sulfur Vacancies: Structure and Catalytic Application. Journal of Physical Chemistry C, 2014, 118, 5346-5351.	1.5	260
47	Postgrowth Tuning of the Bandgap of Single-Layer Molybdenum Disulfide Films by Sulfur/Selenium Exchange. ACS Nano, 2014, 8, 4672-4677.	7.3	101
48	Joined edges in MoS₂: metallic and half-metallic wires. Journal of Physics Condensed Matter, 2013, 25, 312201.	0.7	21
49	Growth of aligned Mo6S6 nanowires on Cu(111). Surface Science, 2013, 611, 1-4.	0.8	20
50	Deactivation of Cu2O(100) by CO Poisoning. Topics in Catalysis, 2013, 56, 1082-1087.	1.3	4
51	Visualization of Compression and Spillover in a Coadsorbed System: Syngas on Cobalt Nanoparticles. ACS Nano, 2013, 7, 4384-4392.	7.3	24
52	Controlled argon beam-induced desulfurization of monolayer molybdenum disulfide. Journal of Physics Condensed Matter, 2013, 25, 252201.	0.7	75
53	The role of van der Waals interaction in the tilted binding of amine molecules to the Au(111) surface. Journal of Physics Condensed Matter, 2012, 24, 222001.	0.7	6
54	Linker-Induced Anomalous Emission of Organic-Molecule Conjugated Metal-Oxide Nanoparticles. ACS Nano, 2012, 6, 4854-4863.	7.3	10

#	Article	IF	Citations
55	Physisorption of nucleobases on graphene: a comparative van der Waals study. Journal of Physics Condensed Matter, 2012, 24, 424210.	0.7	83
56	The Quantum Magnetism of Individual Manganese-12-Acetate Molecular Magnets Anchored at Surfaces. Nano Letters, 2012, 12, 518-521.	4.5	146
57	An MoS_x Structure with High Affinity for Adsorbate Interaction. Angewandte Chemie - International Edition, 2012, 51, 10284-10288.	7.2	13
58	Single layer MoS<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:msub><mml:mrow /><mml:mn>2</mml:mn></mml:msub></mml:math>on the Cu(111) surface: First-principles electronic structure calculations. Physical Review B, 2012, 85, .	1.1	26
59	Dissociative Hydrogen Adsorption on Close-Packed Cobalt Nanoparticle Surfaces. Journal of Physical Chemistry C, 2012, 116, 25868-25873.	1.5	35
60	Toward the Growth of an Aligned Single-Layer MoS₂ Film. Langmuir, 2011, 27, 11650-11653.	1.6	84
61	Effective elastic properties of a van der Waals molecular monolayer at a metal surface. Physical Review B, 2010, 82, .	1.1	18
62	Publisher's Note: Effective elastic properties of a van der Waals molecular monolayer at a metal surface [Phys. Rev. B82, 201410 (2010)]. Physical Review B, 2010, 82, .	1.1	0
63	Reactivity of the Cu2O(1 0 0) surface: Insights from first principles calculations. Surface Science, 2009, 603, 1637-1645.	0.8	70
64	Complete CO Oxidation over Cu2O Nanoparticles Supported on Silica Gel. Nano Letters, 2006, 6, 2095-2098.	4.5	265