

# Duy Le

## List of Publications by Year in descending order

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64  
papers

2,267  
citations

331259

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214527

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docs citations

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times ranked

4509  
citing authors

#	ARTICLE	IF	CITATIONS
1	2Dimensional Transition Metal Dichalcogenides with Tunable Direct Band Gaps: MoS <sub>2</sub> (1-x)Se <sub>2x</sub> Monolayers. Advanced Materials, 2014, 26, 1399-1404.	11.1	334
2	Complete CO Oxidation over Cu <sub>2</sub> O Nanoparticles Supported on Silica Gel. Nano Letters, 2006, 6, 2095-2098.	4.5	265
3	Single-Layer MoS <sub>2</sub> with Sulfur Vacancies: Structure and Catalytic Application. Journal of Physical Chemistry C, 2014, 118, 5346-5351.	1.5	260
4	The Quantum Magnetism of Individual Manganese-12-Acetate Molecular Magnets Anchored at Surfaces. Nano Letters, 2012, 12, 518-521.	4.5	146
5	Postgrowth Tuning of the Bandgap of Single-Layer Molybdenum Disulfide Films by Sulfur/Selenium Exchange. ACS Nano, 2014, 8, 4672-4677.	7.3	101
6	Toward the Growth of an Aligned Single-Layer MoS <sub>2</sub> Film. Langmuir, 2011, 27, 11650-11653.	1.6	84
7	Physisorption of nucleobases on graphene: a comparative van der Waals study. Journal of Physics Condensed Matter, 2012, 24, 424210.	0.7	83
8	Controlled argon beam-induced desulfurization of monolayer molybdenum disulfide. Journal of Physics Condensed Matter, 2013, 25, 252201.	0.7	75
9	Reactivity of the Cu <sub>2</sub> O(1 0 0) surface: Insights from first principles calculations. Surface Science, 2009, 603, 1637-1645.	0.8	70
10	Spin-orbit coupling in the band structure of monolayer WSe <sub>2</sub> . Journal of Physics Condensed Matter, 2015, 27, 182201.	0.7	67
11	Heterogeneous Metal-Free Hydrogenation over Defect-Laden Hexagonal Boron Nitride. ACS Omega, 2016, 1, 1343-1354.	1.6	43
12	Band structure characterization of WS <sub>2</sub> grown by chemical vapor deposition. Applied Physics Letters, 2016, 108, .	1.5	40
13	CO Oxidation Mechanisms on CoO <sub>x</sub> -Pt Thin Films. Journal of the American Chemical Society, 2020, 142, 8312-8322.	6.6	39
14	Dissociative Hydrogen Adsorption on Close-Packed Cobalt Nanoparticle Surfaces. Journal of Physical Chemistry C, 2012, 116, 25868-25873.	1.5	35
15	Two-Dimensional Folding of Polypeptides into Molecular Nanostructures at Surfaces. ACS Nano, 2017, 11, 2420-2427.	7.3	35
16	Structural Stability of N-Alkyl-Functionalized Titanium Metal-Organic Frameworks in Aqueous and Humid Environments. ACS Applied Materials & Interfaces, 2017, 9, 44529-44533.	4.0	33
17	Occupied and unoccupied electronic structure of Na doped MoS <sub>2</sub> (0001). Applied Physics Letters, 2014, 105, .	1.5	30
18	Single layer MoS <sub>2</sub> on the Cu(111) surface: First-principles electronic structure calculations. Physical Review B, 2012, 85, .	1.1	26

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19	High Catalytic Activity of Pd <sub>1</sub> /ZnO(101̄..0) toward Methanol Partial Oxidation: A DFT+KMC Study. ACS Catalysis, 2018, 8, 5553-5569.	5.5	26
20	Mechanically Enhanced Catalytic Reduction of Carbon Dioxide over Defect Hexagonal Boron Nitride. ACS Sustainable Chemistry and Engineering, 2021, 9, 2447-2455.	3.2	25
21	Visualization of Compression and Spillover in a Coadsorbed System: Syngas on Cobalt Nanoparticles. ACS Nano, 2013, 7, 4384-4392.	7.3	24
22	Redox-active ligand controlled selectivity of vanadium oxidation on Au(100). Chemical Science, 2018, 9, 1674-1685.	3.7	24
23	Joined edges in MoS <sub>2</sub> : metallic and half-metallic wires. Journal of Physics Condensed Matter, 2013, 25, 312201.	0.7	21
24	Growth of aligned MoS <sub>6</sub> nanowires on Cu(111). Surface Science, 2013, 611, 1-4.	0.8	20
25	Disorder effect on the anisotropic resistivity of phosphorene determined by a tight-binding model. Physical Review B, 2016, 94, .	1.1	20
26	Effect of Single-Layer MoS <sub>2</sub> on the Geometry, Electronic Structure, and Reactivity of Transition Metal Nanoparticles. Journal of Physical Chemistry C, 2017, 121, 7282-7293.	1.5	20
27	Self-Catalyzed, Low-Temperature Atomic Layer Deposition of Ruthenium Metal Using Zero-Valent Ru(DMBD)(CO) <sub>3</sub> and Water. Chemistry of Materials, 2019, 31, 1304-1317.	3.2	20
28	Effective elastic properties of a van der Waals molecular monolayer at a metal surface. Physical Review B, 2010, 82, .	1.1	18
29	MoS <sub>2</sub> Nanoclusters Grown on TiO <sub>2</sub> : Evidence for New Adsorption Sites at Edges and Sulfur Vacancies. Journal of Physical Chemistry C, 2019, 123, 7185-7201.	1.5	18
30	Metallicity of 2H-MoS <sub>2</sub> induced by Au hybridization. 2D Materials, 2020, 7, 025021.	2.0	17
31	Gold Dispersion and Activation on the Basal Plane of Single-Layer MoS <sub>2</sub> . Journal of Physical Chemistry C, 2018, 122, 267-273.	1.5	16
32	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
33	An MoS <sub>2</sub> Structure with High Affinity for Adsorbate Interaction. Angewandte Chemie - International Edition, 2012, 51, 10284-10288.	7.2	13
34	Adsorbate doping of MoS <sub>2</sub> and WSe <sub>2</sub> : the influence of Na and Co. Journal of Physics Condensed Matter, 2017, 29, 285501.	0.7	12
35	MoS <sub>2</sub> -supported gold nanoparticle for CO hydrogenation. Journal of Physics Condensed Matter, 2017, 29, 415201.	0.7	12
36	CO adsorption on Pd(111) at 0.5ML: A first principles study. Surface Science, 2017, 655, 7-11.	0.8	12

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37	Methoxy Formation Induced Defects on MoS <sub>2</sub> . Journal of Physical Chemistry C, 2018, 122, 10042-10049.	1.5	11
38	A Single Layer of MoS <sub>2</sub> Activates Gold for Room Temperature CO Oxidation on an Inert Silica Substrate. Journal of Physical Chemistry C, 2019, 123, 6592-6598.	1.5	11
39	Characteristics of Single-Molecule Magnet Dimers ([Mn <sub>3</sub> ] <sub>2</sub> ) on Graphene and h-BN. Journal of Physical Chemistry C, 2020, 124, 28186-28200.	1.5	11
40	Anisotropic Properties of Quasi-1D In <sub>4</sub> Se <sub>3</sub> : Mechanical Exfoliation, Electronic Transport, and Polarization-Dependent Photoresponse. Advanced Functional Materials, 2021, 31, 2106459.	7.8	11
41	Linker-Induced Anomalous Emission of Organic-Molecule Conjugated Metal-Oxide Nanoparticles. ACS Nano, 2012, 6, 4854-4863.	7.3	10
42	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
43	Symmetry-resolved surface-derived electronic structure of MoS <sub>2</sub> (001). Journal of Physics Condensed Matter, 2014, 26, 455501.	0.7	9
44	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
45	Effect of monolayer supports on the electronic structure of single-layer MoS <sub>2</sub> . IOP Conference Series: Materials Science and Engineering, 2015, 76, 012011.	0.3	8
46	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
47	The symmetry-resolved electronic structure of 2H-WSe <sub>2</sub> (001). Journal of Physics Condensed Matter, 2016, 28, 345503.	0.7	7
48	Redox Isomeric Surface Structures Are Preferred over Odd-Electron Pt 1+. Chemistry - A European Journal, 2018, 24, 15852-15858.	1.7	7
49	Multi-Electron Reduction Capacity and Multiple Binding Pockets in Metal-Organic Redox Assembly at Surfaces. Chemistry - A European Journal, 2019, 25, 5565-5573.	1.7	7
50	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
51	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
52	Growth of Graphene Nanoflakes/h-BN Heterostructures. Advanced Materials Interfaces, 2021, 8, 2100766.	1.9	5
53	Deactivation of Cu <sub>2</sub> O(100) by CO Poisoning. Topics in Catalysis, 2013, 56, 1082-1087.	1.3	4
54	Fermi surfaces of the topological semimetal CaSn <sub>3</sub> probed through de Haas van Alphen oscillations. Journal of Physics Condensed Matter, 2021, 33, 17LT01.	0.7	4

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55	Pt-dipyridyl tetrazine metal-organic network on the Au(100) surface: insights from first principles calculations. <i>Faraday Discussions</i> , 2017, 204, 83-95.	1.6	4
56	Scattering strength of the scatterer inducing variability in graphene on silicon oxide. <i>Journal of Physics Condensed Matter</i> , 2016, 28, 115301.	0.7	3
57	Catalytic C <sub>2</sub> H <sub>2</sub> synthesis via low temperature CO hydrogenation on defect-rich 2D-MoS <sub>2</sub> and 2D-MoS <sub>2</sub> decorated with Mo clusters. <i>Journal of Chemical Physics</i> , 2020, 152, 074706.	1.2	3
58	Toward alcohol synthesis from CO hydrogenation on Cu(111)-supported MoS <sub>2</sub> – predictions from DFT+KMC. <i>Journal of Chemical Physics</i> , 2021, 154, 174701.	1.2	3
59	Modeling carrier mobility in graphene as a sensitive probe of molecular magnets. <i>Physical Review B</i> , 2021, 103, .	1.1	1
60	On stabilizing spin crossover molecule [Fe(tBu) <sub>2</sub> qsal] <sub>2</sub> on suitable supports: insights from ab initio studies. <i>Journal of Physics Condensed Matter</i> , 2021, 33, 385201.	0.7	1
61	Tailoring the redox capabilities of organic ligands for metal-ligand coordination with vanadium single-sites. <i>Surface Science</i> , 2021, 712, 121888.	0.8	1
62	Methanol carbonylation to acetaldehyde on Au particles supported by single-layer MoS <sub>2</sub> grown on silica. <i>Journal of Physics Condensed Matter</i> , 2022, 34, 104005.	0.7	1
63	Publisher's Note: Effective elastic properties of a van der Waals molecular monolayer at a metal surface [ <i>Phys. Rev. B</i> , 201410 (2010)]. <i>Physical Review B</i> , 2010, 82, .	1.1	0
64	MoS <sub>2</sub> -supported Au <sub>31</sub> for CO hydrogenation: A first-principle study. <i>Journal of Vacuum Science and Technology A: Vacuum, Surfaces and Films</i> , 2020, 38, 032201.	0.9	0