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List of Publications by Year
in descending order

62 papers	4,932 citations	257450 24 h-index	128289 60 g-index
62 all docs	62 docs citations	62 times ranked	6891 citing authors

#	Article	IF	Citations
1	Single-Atom Catalysts Supported by Graphene and Hexagonal Boron Nitride: Structural Stability in the Oxygen Environment. Journal of Physical Chemistry C, 2022, 126, 8637-8644.	3.1	2
2	Field Effect and Local Gating in Nitrogenâ€Terminated Nanopores (NtNP) and Nanogaps (NtNG) in Graphene. ChemPhysChem, 2021, 22, 336-341.	2.1	5
3	First-principles study of nickel reactivity under two-dimensional cover: <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mrow><mml:msub><mml:mi>Ni</mml:mi><mml:mn>2</mml:mn></mml:msub><mml:mathvariant="normal">C</mml:mi></mml:mrow></mml:math> formation at rotated graphene/Ni(111) interface. Physical Review Materials, 2021, 5, .	2.4	0
4	Ab-initio and Monte Carlo study of Fe-based two-dimensional magnets at borophene supported by Ag(111) surface. Physical Review Materials, 2021, 5, .	2.4	0
5	Hydrogen Evolution Reaction over Single-Atom Catalysts Based on Metal Adatoms at Defected Graphene and h-BN. Journal of Physical Chemistry C, 2020, 124, 16860-16867.	3.1	32
6	DNA Sequencing with Single-Stranded DNA Rectification in a Nanogap Gated by N-Terminated Carbon Nanotube Electrodes. ACS Applied Nano Materials, 2020, 3, 3034-3043.	5.0	15
7	Interfacial Charge Transfer Transitions in Colloidal TiO₂ Nanoparticles Functionalized with Salicylic acid and 5-Aminosalicylic acid: A Comparative Photoelectron Spectroscopy and DFT Study. Journal of Physical Chemistry C, 2019, 123, 29057-29066.	3.1	17
8	Formic Acid Synthesis by CO₂ Hydrogenation over Singleâ€Atom Catalysts Based on Ru and Cu Embedded in Graphene. ChemistrySelect, 2018, 3, 2631-2637.	1.5	31
9	Spin Excitations in a <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mn>4</mml:mn><mml:mi>f</mml:mi><mml:mo>â^'</mml:mo><mml:mn>3</mml:mn><mml:mi>d</mml:mi> Heterodimer on MgO. Physical Review Letters, 2018, 121, 257202.	7.8	4
10	Understanding trends in lithium binding at two-dimensional materials. Physical Review Materials, 2018, 2, .	2.4	5
11	Adsorption sites of individual metal atoms on ultrathin MgO(100) films. Physical Review B, 2017, 96, .	3.2	25
12	Graphene/ <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:msub><mml:mi>MoS</mml:mi><mml:mn>2</mml:mn></mml:msub> heterostructures as templates for growing two-dimensional metals: Predictions from ab initio calculations. Physical Review Materials, 2017, 1, .	2.4	13
13	Magnetic remanence in single atoms. Science, 2016, 352, 318-321.	12.6	259
14	Planar versus three-dimensional growth of metal nanostructures at graphene. Carbon, 2016, 96, 216-222.	10.3	7
15	Edge state magnetism in zigzag-interfaced graphene via spin susceptibility measurements. Scientific Reports, 2015, 5, 13382.	3.3	39
16	Electronic and optical properties of reduced graphene oxide. Journal of Materials Chemistry C, 2015, 3, 7632-7641.	5.5	78
17	Collective Diffusion of Gold Clusters and F-Centers at MgO(100) and CaO(100) Surfaces. Journal of Physical Chemistry C, 2014, 118, 28720-28724.	3.1	1
18	Ab initiostudy of structural and electronic properties of partially reduced graphene oxide. Physica Scripta, 2014, T162, 014019.	2.5	9

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19	Atomic Structure, Electronic Properties, and Reactivity of In-Plane Heterostructures of Graphene and Hexagonal Boron Nitride. Journal of Physical Chemistry C, 2014, 118, 16104-16112.	3.1	20
20	Analysis of energy gap opening in graphene oxide. Journal of Physics: Conference Series, 2014, 526, 012003.	0.4	13
21	Binding of atomic oxygen on graphene from small epoxy clusters to a fully oxidized surface. Carbon, 2013, 54, 482-488.	10.3	50
22	Controlling Hydrogenation of Graphene on Ir(111). ACS Nano, 2013, 7, 3823-3832.	14.6	69
23	Magnetism in graphene induced by hydrogen adsorbates. Chemical Physics Letters, 2012, 541, 70-74.	2.6	27
24	Magnetism in nanoscale graphite flakes as seen via electron spin resonance. Physical Review B, 2012, 85, .	3.2	13
25	Linear hydrogen adsorbate structures on graphite induced by self-assembled molecular monolayers. Carbon, 2012, 50, 2052-2056.	10.3	12
26	Electronic properties of the partially hydrogenated armchair carbon nanotubes. Physical Review B, 2011, 84, .	3.2	16
27	Structure and stability of small H clusters on graphene. Physical Review B, 2011, 83, .	3.2	41
28	Bandgap opening in graphene induced by patterned hydrogen adsorption. Nature Materials, 2010, 9, 315-319.	27.5	1,344
29	Effect of adsorbed H atoms on magnetism in monoatomic Fe wires at Ir(100). Physical Review B, 2010, 81, .	3.2	5
30	CO oxidation on fully oxygen covered Ru(0001): Role of step edges. Physical Review B, 2010, 81, .	3.2	23
31	Transition from Mn4+ to Mn3+ induced by surface reconstruction at Î»-MnO2(001). Journal of Chemical Physics, 2010, 133, 204701.	3.0	21
32	Oxidation States of Mn Atoms at Clean and Al₂O₃-Covered LiMn₂O₄(001) Surfaces. Journal of Physical Chemistry C, 2010, 114, 4756-4759.	3.1	73
33	Role of Adsorbed H, C, O, and CO on the Atomic Structure of Free and MgO(100)-Supported Ir₄Clusters: An ab Initio Study. Journal of Physical Chemistry C, 2010, 114, 15653-15660.	3.1	7
34	Nitrogen fixation at passivated Fe nanoclusters supported by an oxide surface: Identification of viable reaction routes using density functional calculations. Physical Review B, 2009, 80, .	3.2	2
35	First-principles study of<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:mi>Î³</mml:mi><mml:msub><mml:mrow><mml:mtext>-Al</mml:mtext></mml:mrow><mml:mn>2</mml:mn></mml:msub></mml:mrow></mml:math> surface. Physical Review B, 2009, 79, .	3.2	48
36	Translational energy and state resolved observations of D and D2 thermally desorbing from D clusters chemisorbed on graphite. Journal of Chemical Physics, 2009, 131, 244707.	3.0	6

#	ARTICLE	IF	CITATIONS
37	Extended atomic hydrogen dimer configurations on the graphite(0001) surface. Journal of Chemical Physics, 2009, 131, 084706.	3.0	80
38	Electronic properties of bilayered manganite<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:msub><mml:mrow><mml:mtext>Ca</mml:mtext></mml:mrow><mml:mrow><mml:mn>2.5</mml:m Physical Review B, 2008, 77, .	3.2	1
39	Electronic properties of an epitaxial silicon oxynitride layer on a 6H-SiC(0001) surface: A first-principles investigation. Applied Physics Letters, 2007, 91, 061930.	3.3	17
40	Probing Enantioselectivity with X-Ray Photoelectron Spectroscopy and Density Functional Theory. Physical Review Letters, 2007, 98, 136102.	7.8	58
41	Effect of Carbon Adsorption on the Isomer Stability of<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:msub><mml:mi>Ir</mml:mi><mml:mn>4</mml:mn></mml:msub></mml:math>Clusters. Physical Review Letters, 2007, 99, 165501.	7.8	16
42	Metastable Structures and Recombination Pathways for Atomic Hydrogen on the Graphite (0001) Surface. Physical Review Letters, 2006, 96, 156104.	7.8	296
43	Clustering of Chemisorbed H(D) Atoms on the Graphite (0001) Surface due to Preferential Sticking. Physical Review Letters, 2006, 97, 186102.	7.8	260
44	PopoviÄ‡etÂal.Reply:. Physical Review Letters, 2006, 96, .	7.8	3
45	Chiral Recognition of Organic Molecules by Atomic Kinks on Surfaces. Physical Review Letters, 2006, 96, 056103.	7.8	120
46	Atomic structure and spin magnetism of self-assembled Co nanowires onPt(332). Physical Review B, 2006, 74, .	3.2	3
47	Supported nanoclusters: Preadsorbates tuning catalytic activity. Physical Review B, 2005, 71, .	3.2	5
48	Sodium PyroxeneNaTiSi2O6: Possible Haldane Spin-1 Chain System. Physical Review Letters, 2004, 93, 036401.	7.8	23
49	Nitrogen adsorption on a supported iron nanocluster. Vacuum, 2004, 74, 173-177.	3.5	2
50	Supported Fe Nanoclusters: Evolution of Magnetic Properties with Cluster Size. Physical Review Letters, 2003, 90, 247202.	7.8	43
51	H2dissociation at defected Cu: Preference for reaction at vacancy and kink sites. Physical Review B, 2002, 65, .	3.2	37
52	MAGNETIC MOMENTS NEAR THE SHARP INTERFACES OF FERROMAGNETIC MATERIALS. International Journal of Modern Physics B, 2002, 16, 3655-3669.	2.0	2
53	Adsorption of O2 and NO on Pd nanocrystals supported on Al2O3/NiAl(): overlayer and edge structures. Surface Science, 2002, 505, 25-38.	1.9	44
54	Oxygen dissociation at close-packed Pt terraces, Pt steps, and Ag-covered Pt steps studied with density functional theory. Surface Science, 2002, 515, 235-244.	1.9	114

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55	Universality in Heterogeneous Catalysis. Journal of Catalysis, 2002, 209, 275-278.	6.2	1,167
56	Density Functional Theory Study of Enantiospecific Adsorption at Chiral Surfaces. Journal of the American Chemical Society, 2002, 124, 14789-14794.	13.7	64
57	Oxygen Dissociation at Pt Steps. Physical Review Letters, 2001, 87, 056103.	7.8	189
58	Distinct Reaction Mechanisms in the Catalytic Oxidation of Carbon Monoxide on Rh(110): Scanning Tunneling Microscopy and Density Functional Theory Studies. Physical Review Letters, 2001, 87, 196104.	7.8	18
59	Magnetic moments of transition metals overlayers on fcc Ni surface. Journal of Physics Condensed Matter, 1998, 10, 8679-8686.	1.8	8
60	Comment on â€œOscillation of the Fe and Co Magnetic Moments near the Sharp(1â^'10)Fe/CoInterfaceâ€• Physical Review Letters, 1998, 80, 1568-1568.	7.8	4
61	Band picture of the spin-Peierls cuprateCuGeO3. Physical Review B, 1997, 56, 4432-4438.	3.2	17
62	Band structure of spin-Peierls cuprate CuGeO3. Journal of Physics Condensed Matter, 1995, 7, 4549-4559.	1.8	14