Catherine Stampfl

List of Publications by Year
in descending order

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267 papers	14,026 citations	20797 60 h-index	25770 108 g-index
272 all docs	272 docs citations	272 times ranked	12931 citing authors

#	Article	IF	Citations
1	Density-functional calculations for III-V nitrides using the local-density approximation and the generalized gradient approximation. Physical Review B, 1999, 59, 5521-5535.	1.1	641
2	Electronic structure and physical properties of early transition metal mononitrides: Density-functional theory LDA, GGA, and screened-exchange LDA FLAPW calculations. Physical Review B, 2001, 63, .	1.1	454
3	Phonon- Versus Electron-Mediated Desorption and Oxidation of CO on Ru(0001). Science, 1999, 285, 1042-1045.	6.0	443
4	Energetics and electronic structure of stacking faults in AlN, GaN, and InN. Physical Review B, 1998, 57, R15052-R15055.	1.1	298
5	Thermodynamic stability and structure of copper oxide surfaces: A first-principles investigation. Physical Review B, 2007, 75, .	1.1	275
6	Oxygen adsorption on Ag(111): A density-functional theory investigation. Physical Review B, 2002, 65, .	1.1	256
7	Converged properties of clean metal surfaces by all-electron first-principles calculations. Surface Science, 2006, 600, 703-715.	0.8	252
8	Oxygen adsorption and stability of surface oxides onCu(111): A first-principles investigation. Physical Review B, 2006, 73, .	1.1	248
9	Water adsorption on the stoichiometric and reduced CeO2(111) surface: a first-principles investigation. Physical Chemistry Chemical Physics, 2009, 11, 9188.	1.3	229
10	Theoretical investigation of native defects, impurities, and complexes in aluminum nitride. Physical Review B, 2002, 65, .	1.1	225
11	Structure and Stability of a High-Coverage(1Ã—1)Oxygen Phase on Ru(0001). Physical Review Letters, 1996, 77, 3371-3374.	2.9	220
12	Role of Embedded Clustering in Dilute Magnetic Semiconductors: Cr Doped GaN. Physical Review Letters, 2005, 95, 256404.	2.9	212
13	Native defects and impurities in InN: First-principles studies using the local-density approximation and self-interaction and relaxation-corrected pseudopotentials. Physical Review B, 2000, 61, R7846-R7849.	1.1	209
14	Robotics, Smart Wearable Technologies, and Autonomous Intelligent Systems for Healthcare During the COVIDâ€19 Pandemic: An Analysis of the State of the Art and Future Vision. Advanced Intelligent Systems, 2020, 2, 2000071.	3.3	204
15	Theory of doping and defects in IIIâ€“V nitrides. Journal of Crystal Growth, 1998, 189-190, 505-510.	0.7	202
16	Catalysis and corrosion: the theoretical surface-science context. Surface Science, 2002, 500, 368-394.	0.8	197
17	First-Principles Theory of Surface Thermodynamics and Kinetics. Physical Review Letters, 1999, 83, 2993-2996.	2.9	181
18	Why is a Noble Metal Catalytically Active? The Role of the O-Ag Interaction in the Function of Silver as an Oxidation Catalyst. Physical Review Letters, 2003, 90, 256102.	2.9	178

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19	Insights into the function of silver as an oxidation catalyst byab initioatomistic thermodynamics. Physical Review B, 2003, 68, .	1.1	178
20	Adsorption of Xe Atoms on Metal Surfaces: New Insights from First-Principles Calculations. Physical Review Letters, 2003, 90, 066104.	2.9	168
21	First-principles investigation of quantum emission from hBN defects. Nanoscale, 2017, 9, 13575-13582.	2.8	167
22	Role of Subsurface Oxygen in Oxide Formation at Transition Metal Surfaces. Physical Review Letters, 2002, 89, 096103.	2.9	166
23	Surface core-level shifts of clean and oxygen-covered Ru(0001). Physical Review B, 2001, 63, .	1.1	163
24	Identification of stable and metastable adsorption sites of K adsorbed on Al(111). Physical Review Letters, 1992, 69, 1532-1535.	2.9	161
25	Theoretical study of O adlayers on Ru(0001). Physical Review B, 1996, 54, 2868-2872.	1.1	160
26	Stability and morphology of cerium oxide surfaces in an oxidizing environment: A first-principles investigation. Journal of Chemical Physics, 2009, 131, .	1.2	150
27	Doping of AlxGa1â^'xN. Applied Physics Letters, 1998, 72, 459-461.	1.5	149
28	Subsurface oxygen and surface oxide formation at Ag(111): A density-functional theory investigation. Physical Review B, 2003, 67, .	1.1	135
29	Density functional study of oxygen on Cu(100) and Cu(110) surfaces. Physical Review B, 2010, 81, .	1.1	130
30	High-Fidelity Bilateral Teleoperation Systems and the Effect of Multimodal Haptics. IEEE Transactions on Systems, Man, and Cybernetics, 2007, 37, 1512-1528.	5.5	127
31	Cohesive properties of group-III nitrides: A comparative study of all-electron and pseudopotential calculations using the generalized gradient approximation. Physical Review B, 2002, 65, .	1.1	126
32	Superhard Nitride-Based Nanocomposites: Role of Interfaces and Effect of Impurities. Physical Review Letters, 2006, 97, 086102.	2.9	122
33	Anomalous Behavior of Ru for Catalytic Oxidation: A Theoretical Study of the Catalytic ReactionCO+12O2â†'CO2. Physical Review Letters, 1997, 78, 1500-1503.	2.9	121
34	Atomistic description of oxide formation on metal surfaces: the example of ruthenium. Chemical Physics Letters, 2002, 352, 311-317.	1.2	120
35	Metastable precursors during the oxidation of the Ru(0001) surface. Physical Review B, 2002, 65, .	1.1	119
36	First-principles investigations of the structure and stability of oxygen adsorption and surface oxide formation at Au(111). Physical Review B, 2007, 76, .	1.1	119

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37	A first-principles study of the effects of atom impurities, defects, strain, electric field and layer thickness on the electronic and magnetic properties of the C2N nanosheet. Carbon, 2020, 157, 371-384.	5.4	114
38	Native defect-induced multifarious magnetism in nonstoichiometric cuprous oxide: First-principles study of bulk and surface properties of<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:msub><mml:mrow><mml:mtext>Cu</mml:mtext></mml:mrow><mml:mrow><mml:mn>2</mml:mn></mml:mr Physical Review B, 2009, 79, .	1.1	109
39	Surface processes and phase transitions from ab initio atomistic thermodynamics and statistical mechanics. Catalysis Today, 2005, 105, 17-35.	2.2	108
40	Magnetic Metastability in Tetrahedrally Bonded Magnetic III-Nitride Semiconductors. Physical Review Letters, 2006, 97, 016402.	2.9	105
41	Thermodynamic and spectroscopic properties of oxygen on silver under an oxygen atmosphere. Physical Chemistry Chemical Physics, 2015, 17, 9288-9312.	1.3	103
42	Properties of the gold oxidesAu2O3andAu2O: First-principles investigation. Physical Review B, 2007, 75, .	1.1	101
43	BrÃnsted acid sites based on penta-coordinated aluminum species. Nature Communications, 2016, 7, 13820.	5.8	99
44	Metallic to insulating nature ofTaNx:â€,Role of Ta and N vacancies. Physical Review B, 2003, 67, .	1.1	98
45	Hydrogen adsorption capacity of adatoms on double carbon vacancies of graphene: A trend study from first principles. Physical Review B, 2013, 87, .	1.1	98
46	Stable and metastable structures of the multiphase tantalum nitride system. Physical Review B, 2005, 71, .	1.1	97
47	Xe adsorption on metal surfaces: First-principles investigations. Physical Review B, 2005, 72, .	1.1	94
48	Geometry and diameter dependence of the electronic and physical properties of GaN nanowires from first principles. Physical Review B, 2008, 77, .	1.1	88
49	The role of titanium nitride supports for single-atom platinum-based catalysts in fuel cell technology. Physical Chemistry Chemical Physics, 2012, 14, 16552.	1.3	88
50	Alloy Catalyst in a Reactive Environment: The Example of Ag-Cu Particles for Ethylene Epoxidation. Physical Review Letters, 2010, 104, 035503.	2.9	86
51	THEORY OF ALKALI-METAL ADSORPTION ON CLOSE-PACKED METAL SURFACES. Surface Review and Letters, 1995, 02, 317-343.	0.5	76
52	LEED structural analysis of Al(111)-K-(âˆš3 Ã— âˆš3)R30Â°: Identification of stable and metastable adsorption sites. Physical Review B, 1994, 49, 4959-4972.	1.1	74
53	First-principles investigation of nonmetal doped single-layer BiOBr as a potential photocatalyst with a low recombination rate. Physical Chemistry Chemical Physics, 2020, 22, 15354-15364.	1.3	74
54	Insights into the Electronic Structure of the Oxygen Species Active in Alkene Epoxidation on Silver. ACS Catalysis, 2015, 5, 5846-5850.	5.5	71

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55	Evaluation of van der Waals density functionals for layered materials. Physical Review Materials, 2018, 2, .	0.9	71
56	Hardness analysis of cubic metal mononitrides from first principles. Physical Review B, 2012, 85, .	1.1	70
57	Structure and properties ofTiN(111)âˆ•SixNyâˆ•TiN(111)interfaces in superhard nanocomposites: First-principles investigations. Physical Review B, 2006, 74, .	1.1	69
58	Cooperation of Ni and CaO at Interface for CO₂ Reforming of CH₄: A Combined Theoretical and Experimental Study. ACS Catalysis, 2019, 9, 10060-10069.	5.5	68
59	The DNA-binding Domain of the Hexameric Arginine Repressor. Journal of Molecular Biology, 1995, 254, 150-162.	2.0	67
60	A Dirac-semimetal two-dimensional BeN4: Thickness-dependent electronic and optical properties. Applied Physics Letters, 2021, 118, .	1.5	64
61	Alkali-metal adsorption on Al(111) and Al(100). Surface Science, 1994, 307-309, 8-15.	0.8	62
62	Surface oxides of the oxygenâ€“copper system: Precursors to the bulk oxide phase?. Surface Science, 2007, 601, 5809-5813.	0.8	60
63	Trends in adsorption of noble gases He, Ne, Ar, Kr, and Xe on<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:mi mathvariant="normal">Pd</mml:mi><mml:mrow><mml:mo>(</mml:mo><mml:mn>111</mml:mn><mml:mo>)</mml:mo></mml:mrow> All-electron d. Physical Review B, 2008, 77, .	1.1	59
64	Codoping of aluminum and gallium with nitrogen in ZnO: A comparative first-principles investigation. Physical Review B, 2009, 79, .	1.1	59
65	Density-functional theory study of the catalytic oxidation of CO over transition metal surfaces. Surface Science, 1999, 433-435, 119-126.	0.8	58
66	Mechanism and control of the metal-to-insulator transition in rocksalt tantalum nitride. Physical Review B, 2002, 65, .	1.1	57
67	Structural analysis of the two c(2 Ã— 2) phases of Na adsorbed on Al(100). Surface Science, 1995, 330, 182-192.	0.8	55
68	Efficient Prediction of Structural and Electronic Properties of Hybrid 2D Materials Using Complementary DFT and Machine Learning Approaches. Advanced Theory and Simulations, 2019, 2, 1800128.	1.3	55
69	Magnetism of Co-doped ZnO epitaxially grown on a ZnO substrate. Physical Review B, 2012, 85, .	1.1	54
70	Sensing sulfur-containing gases using titanium and tin decorated zigzag graphene nanoribbons from first-principles. Physical Chemistry Chemical Physics, 2015, 17, 6925-6932.	1.3	54
71	Low-energy electron-diffraction analysis of the (âˆš7 Ã— âˆš7)R19.1Â°-S adsorbate structure on the Pd(111) surface. Surface Science, 1994, 317, 84-98.	0.8	52
72	Theoretical analysis of the electronic structure of the stable and metastablec(2Ã—2)phases of Na on Al(001): Comparison with angle-resolved ultraviolet photoemission spectra. Physical Review B, 1998, 57, 15251-15260.	1.1	52

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73	Formation and Structural Analysis of a Surface Alloy: Al(111)-(2 Ã— 2)-Na. Physical Review Letters, 1995, 74, 1617-1620.	2.9	51
74	Stability, structure, and electronic properties of chemisorbed oxygen and thin surface oxides on Ir(111). Physical Review B, 2008, 78, .	1.1	51
75	Shape and surface structure of gold nanoparticles under oxidizing conditions. Physical Review B, 2008, 77, .	1.1	49
76	Control of C₃N₄and C₄N₃carbon nitride nanosheetsâ€™ electronic and magnetic properties through embedded atoms. Physical Chemistry Chemical Physics, 2020, 22, 2249-2261.	1.3	49
77	Strain, electric-field and functionalization induced widely tunable electronic properties in MoS₂/BC ₃, /C ₃ N and /$C_{3}N_{4}$ van der Waals heterostructures. Nanotechnology, 2020, 31, 295202.	1.3	48
78	Effect of electric field and vertical strain on the electro-optical properties of the MoSi2N4 bilayer: A first-principles calculation. Journal of Applied Physics, 2021, 129, .	1.1	48
79	Surface properties of the refractory metal-nitride semiconductor ScN: Screened-exchange LDA-FLAPW investigations. Physical Review B, 2002, 65, .	1.1	47
80	Neutral and charged embedded clusters of Mn in doped GaN from first principles. Physical Review B, 2007, 76, .	1.1	46
81	Role of oxygen inTiN(111)âˆ•SixNyâˆ•TiN(111)interfaces: Implications for superhard nanocrystallinencâˆ’TiNâˆ•aâˆ’Si3N4nanocomposites. Physical Review B, 2006, 74, .	1.1	45
82	Mechanical properties of zirconia, doped and undoped yttria-stabilized cubic zirconia from first-principles. Journal of Physics and Chemistry of Solids, 2018, 122, 51-71.	1.9	45
83	Nitrogen vacancies in InN: Vacancy clustering and metallic bonding from first principles. Physical Review B, 2008, 77, .	1.1	43
84	First-principles investigation of Ag-Cu alloy surfaces in an oxidizing environment. Physical Review B, 2008, 77, .	1.1	43
85	Ab initiolattice dynamics and thermal expansion of<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:msub><mml:mrow><mml:mtext>Cu</mml:mtext></mml:mrow><mml:mn>2</mml:mn></mml:msu Physical Review B, 2009, 80, .	1.1	43
86	Band gap engineering of wurtzite and zinc-blende GaN/AlN superlattices from first principles. Journal of Applied Physics, 2010, 108, .	1.1	43
87	Magic numbers of nanoholes in graphene: Tunable magnetism and semiconductivity. Physical Review B, 2011, 84, .	1.1	43
88	Multiple CO₂ capture in stable metal-doped graphene: a theoretical trend study. RSC Advances, 2015, 5, 50975-50982.	1.7	42
89	Half-Metallicity and Efficient Spin Injection inAlN/GaNâˆ¶Cr(0001) Heterostructure. Physical Review Letters, 2005, 94, 146602.	2.9	41
90	Embedded clustering in Cr-doped AlN: Evidence for general behavior in dilute magnetic III-nitride semiconductors. Journal of Applied Physics, 2007, 101, 103917.	1.1	40

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91	Structure and stability of transition metal nitride interfaces from first-principles: AlN/VN, AlN/TiN, and VN/TiN. Applied Surface Science, 2012, 258, 5638-5645.	3.1	40
92	First principles study of 3d transition metal doped <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" altimg="si0020.gif" overflow="scroll"><mml:msub><mml:mrow><mml:mi>Cu</mml:mi></mml:mrow><mml:mrow><mml:mn>3</mml:mn></mml:mrow></mml:msub><mml:mrow><mml:mi mathvariant="normal">N</mml:mi></mml:mrow></mml:math>. Journal of Magnetism and Magnetic Materials, 2012, 324, 3138-3143.	1.0	40
93	Hybrid functional calculations of point defects and hydrogen in<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:msub><mml:mi mathvariant="normal">SrZrO</mml:mi><mml:mn>3</mml:mn></mml:msub></mml:math>. Physical Review B, 2014, 89, .	1.1	40
94	Exploiting the Novel Electronic and Magnetic Structure of C₃N via Functionalization and Conformation. Advanced Electronic Materials, 2019, 5, 1900459.	2.6	40
95	Band-gap control of graphenelike borocarbonitride <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mrow><mml:mi>g</mml:mi><mml:mtext>â^’</mml:mtext><mml:msub><mml:mi mathvariant="normal">N</mml:mi></mml:mrow></mml:math> bilayers by electrical gating. Physical Review B, 2020, 102, .	1.1	40
96	Nitrogen adsorption and thin surface nitrides on Cu(111) from first-principles. Surface Science, 2007, 601, 4775-4785.	0.8	39
97	Resolving Deactivation Pathways of Co Porphyrin-Based Electrocatalysts for CO₂ Reduction in Aqueous Medium. ACS Catalysis, 2021, 11, 3715-3729.	5.5	39
98	Energy barriers and chemical properties in the coadsorption of carbon monoxide and oxygen on Ru(0001). Physical Review B, 2002, 65, .	1.1	38
99	Spatial distribution and magnetism in poly-Cr-doped GaN from first principles. Physical Review B, 2007, 75, .	1.1	38
100	Morphology of copper nanoparticles in a nitrogen atmosphere: A first-principles investigation. Physical Review B, 2008, 77, .	1.1	38
101	Multiferroic crossover in perovskite oxides. Physical Review B, 2016, 93, .	1.1	38
102	Embedding of atoms into the nanopore sites of the C₆N₆and C₆N₈porous carbon nitride monolayers with tunable electronic properties. Physical Chemistry Chemical Physics, 2020, 22, 6418-6433.	1.3	38
103	The Electronic, Optical, and Thermoelectric Properties of Monolayer PbTe and the Tunability of the Electronic Structure by External Fields and Defects. Physica Status Solidi (B): Basic Research, 2020, 257, 2000182.	0.7	38
104	Machine learning the band gap properties of kesterite <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:msub><mml:mi mathvariant="normal">I</mml:mi><mml:mn>2</mml:mn></mml:msub><mml:mtext>â^’</mml:mtext><mml:mi>II</mml:mi><mml:msub><mml:mi mathvariant="normal">V</mml:mi><mml:mn>4</mml:mn></mml:msub></mml:math> quaternary compounds for photovoltaics applications. Physical Review Materials, 2018, 2, .	0.9	38
105	Doping of AlxGa1â^’xN alloys. Materials Science and Engineering B: Solid-State Materials for Advanced Technology, 1999, 59, 253-257.	1.7	37
106	Theory of Adsorption on Metal Substrates. Handbook of Surface Science, 2000, , 285-356.	0.3	37
107	Agâ€“Cu alloy surfaces in an oxidizing environment: A first-principles study. Surface Science, 2009, 603, 1467-1475.	0.8	37
108	Built-in electric fields and valence band offsets in InN/GaN(0001) superlattices: First-principles investigations. Journal of Applied Physics, 2011, 109, .	1.1	36

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109	Unravelling the effects of layered supports on Ru nanoparticles for enhancing N2 reduction in photocatalytic ammonia synthesis. Applied Catalysis B: Environmental, 2019, 259, 118026.	10.8	36
110	Acidity enhanced [Al]MCM-41 via ultrasonic irradiation for the Beckmann rearrangement of cyclohexanone oxime to É›-caprolactam. Journal of Catalysis, 2018, 358, 71-79.	3.1	35
111	Boron-Doped g-C₆N₆ Layer as a Metal-Free Photoelectrocatalyst for N₂ Reduction Reaction. Journal of Physical Chemistry C, 2019, 123, 28739-28743.	1.5	35
112	Vacancies and interstitials in indium nitride: Vacancy clustering and molecular bondlike formation from first principles. Physical Review B, 2009, 79, .	1.1	34
113	Defect complexes and cluster doping of InN: First-principles investigations. Physical Review B, 2009, 79, .	1.1	34
114	A Firstâ€Principles Study of C₃N Nanostructures: Control and Engineering of the Electronic and Magnetic Properties of Nanosheets, Tubes and Ribbons. ChemPhysChem, 2020, 21, 164-174.	1.0	34
115	Dirac half-metallicity of Thin PdCl3 Nanosheets: Investigation of the Effects of External Fields, Surface Adsorption and Defect Engineering on the Electronic and Magnetic Properties. Scientific Reports, 2020, 10, 213.	1.6	33
116	Theoretical identification of a (2 Ã— 2) composite double layer ordered surface alloy of Na on Al(111). Surface Science, 1994, 319, L23-L28.	0.8	32
117	Atomic and electronic structure of single and multiple vacancies in GaN nanowires from first-principles. Physical Review B, 2009, 79, .	1.1	32
118	Environment-dependent nanomorphology of TiN: the influence of surface vacancies. Nanoscale, 2012, 4, 5183.	2.8	32
119	Two-dimensional Janus semiconductor BiTeCl and BiTeBr monolayers: a first-principles study on their tunable electronic properties via an electric field and mechanical strain. Physical Chemistry Chemical Physics, 2021, 23, 15216-15223.	1.3	32
120	A first-principles density functional study of chlorophenol adsorption on Cu2O(110):CuO. Journal of Chemical Physics, 2009, 130, 184505.	1.2	30
121	Cu/ZnO(0001) under oxidating and reducing conditions: A first-principles survey of surface structures. Physical Review B, 2011, 84, .	1.1	30
122	Real Time Determination of the Electronic Structure of Unstable Reaction Intermediates during Au₂O₃ Reduction. Journal of Physical Chemistry Letters, 2014, 5, 80-84.	2.1	30
123	Strongly enhanced acidity and activity of amorphous silicaâ€“alumina by formation of pentacoordinated AlV species. Journal of Catalysis, 2019, 372, 1-7.	3.1	30
124	Doping of AlGaN Alloys. MRS Internet Journal of Nitride Semiconductor Research, 1999, 4, 890-901.	1.0	29
125	Reaction intermediates of methanol synthesis and the waterâ€“gas-shift reaction on the ZnO(0001) surface. Surface Science, 2010, 604, 1742-1751.	0.8	29
126	Oxygen adsorption on the (1 Ã— 1) and (2 Ã— 1) reconstructed C(111) surfaces: a density functional theory study. Journal of Physics Condensed Matter, 2010, 22, 265007.	0.7	29

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127	Playing with Dimensions: Rational Design for Heteroepitaxial pâ€“n Junctions. Nano Letters, 2012, 12, 68-76.	4.5	29
128	Oxygen Vacancies in the Single Layer of Ti₂CO₂ MXene: Effects of Gating Voltage, Mechanical Strain, and Atomic Impurities. Physica Status Solidi (B): Basic Research, 2020, 257, 2000343.	0.7	29
129	Nature of Xenon adsorption on graphite: On-top versus hollow site preference. Physical Review B, 2007, 76, .	1.1	28
130	Active sites and mechanism of the direct conversion of methane and carbon dioxide to acetic acid over the zinc-modified H-ZSM-5 zeolite. Catalysis Science and Technology, 2019, 9, 6297-6307.	2.1	28
131	THEORETICAL EVIDENCE FOR UNUSUAL BONDING GEOMETRY AND PHASE TRANSITIONS OF Na ON Al(001). Surface Review and Letters, 1994, 01, 213-219.	0.5	27
132	Bridging the temperature and pressure gaps: close-packed transition metal surfaces in an oxygen environment. Journal of Physics Condensed Matter, 2008, 20, 184021.	0.7	27
133	Mitigation of CO poisoning on functionalized Ptâ€“TiN surfaces. Physical Chemistry Chemical Physics, 2013, 15, 19450.	1.3	27
134	Structural and electronic properties of<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:msub><mml:mi>SrZrO</mml:mi><mml:mn>3</mml:mn></mml:msub></m Sr(Ti,Zr)<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:msub><mml:mi mathvariant="normal">O</mml:mi><mml:mn>3</mml:mn></mml:msub></mml:math>alloys. Physical Review B, 2015, 92, .	1.1	27
135	Design of shallow acceptors in ZnO through early transition metals codoped with N acceptors. Physical Review B, 2011, 83, .	1.1	26
136	Density-Functional Prediction of a Surface Magnetic Phase in<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:msub><mml:mrow><mml:mi>SrTiO</mml:mi></mml:mrow><mml:mrow><mml:mn>3</mml:mn></</ Induced by Al Vacancies. Physical Review Letters, 2014, 113, 186401.	2.9	26
137	Hydrogen Adsorption on Nearly Zigzag-Edged Nanoribbons: A Density Functional Theory Study. Scientific Reports, 2017, 7, 15727.	1.6	26
138	Defects and Defect Reactions in Semiconductor Nitrides. Acta Physica Polonica A, 1999, 96, 613-627.	0.2	25
139	Phase diagram of O/Ru(0001) from first principles. Chemical Physics Letters, 2002, 361, 317-320.	1.2	23
140	Continuously tunable band gap in GaN/AlN (0001) superlattices via built-in electric field. Physical Review B, 2010, 81, .	1.1	23
141	Acceptor doping in the proton conductor SrZrO₃. Physical Chemistry Chemical Physics, 2017, 19, 11485-11491.	1.3	23
142	Case Report: Utilizing AI and NLP to Assist with Healthcare and Rehabilitation During the COVID-19 Pandemic. Frontiers in Artificial Intelligence, 2021, 4, 613637.	2.0	23
143	Band-gap engineering, magnetic behavior and Dirac-semimetal character in the MoSi₂N₄ nanoribbon with armchair and zigzag edges. Journal Physics D: Applied Physics, 2022, 55, 035301.	1.3	23
144	First-principles study of the mechanism of ethylene epoxidation over Agâ€“Cu particles. Journal of Materials Chemistry, 2010, 20, 10521.	6.7	22

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145	A first-principles study of ultrathin nanofilms of MgO-supported TiN. Physical Chemistry Chemical Physics, 2012, 14, 2462.	1.3	22
146	A new LEED investigation of the Cu(110)-(2 Ã— 3)N structure. Surface Science, 1997, 381, L589-L593.	0.8	21
147	van der Waals Forces Control the Internal Chemical Structure of Monolayers within the Lamellar Materials CuInP₂S₆ and CuBiP₂Se₆. Journal of Physical Chemistry C, 2018, 122, 22675-22687.	1.5	21
148	First-principles design of bifunctional oxygen reduction and evolution catalysts through bimetallic centers in metalâ€“organic frameworks. Catalysis Science and Technology, 2018, 8, 3666-3674.	2.1	21
149	Composition-structure-function correlation of Ca/Zn/AlOx catalysts for the ketonization of acetic acid. Catalysis Today, 2020, 351, 58-67.	2.2	21
150	Exceptional in-plane and interfacial thermal transport in graphene/2D-SiC van der Waals heterostructures. Scientific Reports, 2020, 10, 22050.	1.6	21
151	Density of Configurational States from First-Principles Calculations: The Phase Diagram of Al-Na Surface Alloys. ChemPhysChem, 2005, 6, 1923-1928.	1.0	20
152	Microscopic origin of<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mi>n</mml:mi></mml:math>-type behavior in Si-doped AlN. Physical Review B, 2013, 88, .	1.1	20
153	Benzylation of Arenes with Benzyl Chloride over H-Beta Zeolite: Effects from Acidity and Shape-Selectivity. Journal of Physical Chemistry C, 2017, 121, 15248-15255.	1.5	20
154	High mobility in Î±-phosphorene isostructures with low deformation potential. Physical Chemistry Chemical Physics, 2020, 22, 2276-2282.	1.3	20
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