Catherine Stampfl

List of Publications by Citations

256 papers	11,830 citations	57 h-index	100 g-index
272 ext. papers	12,920 ext. citations	4.3 avg, IF	6.67 L-index

#	Paper	IF	Citations
256	Density-functional calculations for III-V nitrides using the local-density approximation and the generalized gradient approximation. *Physical Review B*, **1999**, 59, 5521-5535	3.3	564
255	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,	3.3	410
254	Phonon- versus electron-mediated desorption and oxidation of CO on Ru(0001). *Science*, **1999**, 285, 1042-5	33	395
253	Energetics and electronic structure of stacking faults in AlN, GaN, and InN. *Physical Review B*, **1998**, 57, R15052-R15055	3.3	273
252	Thermodynamic stability and structure of copper oxide surfaces: A first-principles investigation. *Physical Review B*, **2007**, 75,	3.3	247
251	Oxygen adsorption on Ag(111): A density-functional theory investigation. *Physical Review B*, **2002**, 65,	3.3	231
250	Converged properties of clean metal surfaces by all-electron first-principles calculations. *Surface Science*, **2006**, 600, 703-715	1.8	225
249	Oxygen adsorption and stability of surface oxides on Cu(111): A first-principles investigation. *Physical Review B*, **2006**, 73,	3.3	216
248	Structure and Stability of a High-Coverage (1 x 1) Oxygen Phase on Ru(0001). *Physical Review Letters*, **1996**, 77, 3371-3374	7.4	209
247	Water adsorption on the stoichiometric and reduced CeO2(111) surface: a first-principles investigation. *Physical Chemistry Chemical Physics*, **2009**, 11, 9188-99	3.6	198
246	Theoretical investigation of native defects, impurities, and complexes in aluminum nitride. *Physical Review B*, **2002**, 65,	3.3	196
245	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	3.3	196
244	Role of embedded clustering in dilute magnetic semiconductors: Cr doped GaN. *Physical Review Letters*, **2005**, 95, 256404	7.4	189
243	Catalysis and corrosion: the theoretical surface-science context. *Surface Science*, **2002**, 500, 368-394	1.8	186
242	Theory of doping and defects in III-V nitrides. *Journal of Crystal Growth*, **1998**, 189-190, 505-510	1.6	175
241	First-Principles Theory of Surface Thermodynamics and Kinetics. *Physical Review Letters*, **1999**, 83, 2993-2996	7.4	166
240	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	7.4	158

239	Adsorption of Xe atoms on metal surfaces: new insights from first-principles calculations. *Physical Review Letters*, **2003**, 90, 066104	7.4	158
238	Insights into the function of silver as an oxidation catalyst by ab initio atomistic thermodynamics. *Physical Review B*, **2003**, 68,	3.3	157
237	Role of subsurface oxygen in oxide formation at transition metal surfaces. *Physical Review Letters*, **2002**, 89, 096103	7.4	154
236	Identification of stable and metastable adsorption sites of K adsorbed on Al(111). *Physical Review Letters*, **1992**, 69, 1532-1535	7.4	153
235	Theoretical study of O adlayers on Ru(0001). *Physical Review B*, **1996**, 54, 2868-2872	3.3	147
234	Surface core-level shifts of clean and oxygen-covered Ru(0001). *Physical Review B*, **2001**, 63,	3.3	144
233	Stability and morphology of cerium oxide surfaces in an oxidizing environment: A first-principles investigation. *Journal of Chemical Physics*, **2009**, 131, 104701	3.9	129
232	Doping of AlxGa1□N. *Applied Physics Letters*, **1998**, 72, 459-461	3.4	129
231	Subsurface oxygen and surface oxide formation at Ag(111): A density-functional theory investigation. *Physical Review B*, **2003**, 67,	3.3	127
230	First-principles investigation of quantum emission from hBN defects. *Nanoscale*, **2017**, 9, 13575-13582	7.7	122
229	Density functional study of oxygen on Cu(100) and Cu(110) surfaces. *Physical Review B*, **2010**, 81,	3.3	118
228	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,	3.3	118
227	Anomalous Behavior of Ru for Catalytic Oxidation: A Theoretical Study of the Catalytic Reaction CO+12O2-ĊO2. *Physical Review Letters*, **1997**, 78, 1500-1503	7.4	115
226	Superhard nitride-based nanocomposites: role of interfaces and effect of impurities. *Physical Review Letters*, **2006**, 97, 086102	7.4	114
225	Robotics, Smart Wearable Technologies, and Autonomous Intelligent Systems for Healthcare During the COVID-19 Pandemic: An Analysis of the State of the Art and Future Vision. *Advanced Intelligent Systems*, **2020**, 2, 2000071	6	113
224	Metastable precursors during the oxidation of the Ru(0001) surface. *Physical Review B*, **2002**, 65,	3.3	112
223	Atomistic description of oxide formation on metal surfaces: the example of ruthenium. *Chemical Physics Letters*, **2002**, 352, 311-317	2.5	111
222	First-principles investigations of the structure and stability of oxygen adsorption and surface oxide formation at Au(111). *Physical Review B*, **2007**, 76,	3.3	110

221	Magnetic metastability in tetrahedrally bonded magnetic III-nitride semiconductors. *Physical Review Letters*, **2006**, 97, 016402	7.4	98
220	Surface processes and phase transitions from ab initio atomistic thermodynamics and statistical mechanics. *Catalysis Today*, **2005**, 105, 17-35	5.3	98
219	High-fidelity bilateral teleoperation systems and the effect of multimodal haptics. *IEEE Transactions on Systems, Man, and Cybernetics*, **2007**, 37, 1512-28		97
218	Native defect-induced multifarious magnetism in nonstoichiometric cuprous oxide: First-principles study of bulk and surface properties of Cu2O. *Physical Review B*, **2009**, 79,	3.3	96
217	Metallic to insulating nature of TaNx: Role of Ta and N vacancies. *Physical Review B*, **2003**, 67,	3.3	94
216	Xe adsorption on metal surfaces: First-principles investigations. *Physical Review B*, **2005**, 72,	3.3	90
215	Properties of the gold oxides Au2O3 and Au2O: First-principles investigation. *Physical Review B*, **2007**, 75,	3.3	89
214	Stable and metastable structures of the multiphase tantalum nitride system. *Physical Review B*, **2005**, 71,	3.3	86
213	Hydrogen adsorption capacity of adatoms on double carbon vacancies of graphene: A trend study from first principles. *Physical Review B*, **2013**, 87,	3.3	85
212	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	10.4	81
211	Alloy catalyst in a reactive environment: the example of ag-cu particles for ethylene epoxidation. *Physical Review Letters*, **2010**, 104, 035503	7.4	80
210	Geometry and diameter dependence of the electronic and physical properties of GaN nanowires from first principles. *Physical Review B*, **2008**, 77,	3.3	77
209	The role of titanium nitride supports for single-atom platinum-based catalysts in fuel cell technology. *Physical Chemistry Chemical Physics*, **2012**, 14, 16552-7	3.6	75
208	LEED structural analysis of Al(111)-K-(sqrt 3 x sqrt 3)R30 degrees: Identification of stable and metastable adsorption sites. *Physical Review B*, **1994**, 49, 4959-4972	3.3	73
207	Brønsted acid sites based on penta-coordinated aluminum species. *Nature Communications*, **2016**, 7, 13820	17.4	73
206	Thermodynamic and spectroscopic properties of oxygen on silver under an oxygen atmosphere. *Physical Chemistry Chemical Physics*, **2015**, 17, 9288-312	3.6	70
205	THEORY OF ALKALI-METAL ADSORPTION ON CLOSE-PACKED METAL SURFACES. *Surface Review and Letters*, **1995**, 02, 317-343	1.1	70
204	Structure and properties of TiN(111)/SixNy/TiN(111) interfaces in superhard nanocomposites: First-principles investigations. *Physical Review B*, **2006**, 74,	3.3	66

203	Hardness analysis of cubic metal mononitrides from first principles. *Physical Review B*, **2012**, 85,	3.3	63
202	Alkali-metal adsorption on Al(111) and Al(100). *Surface Science*, **1994**, 307-309, 8-15	1.8	61
201	Insights into the Electronic Structure of the Oxygen Species Active in Alkene Epoxidation on Silver. *ACS Catalysis*, **2015**, 5, 5846-5850	13.1	59
200	Codoping of aluminum and gallium with nitrogen in ZnO: A comparative first-principles investigation. *Physical Review B*, **2009**, 79,	3.3	58
199	Surface oxides of the oxygen□opper system: Precursors to the bulk oxide phase?. *Surface Science*, **2007**, 601, 5809-5813	1.8	57
198	Density-functional theory study of the catalytic oxidation of CO over transition metal surfaces. *Surface Science*, **1999**, 433-435, 119-126	1.8	55
197	Mechanism and control of the metal-to-insulator transition in rocksalt tantalum nitride. *Physical Review B*, **2002**, 65,	3.3	54
196	The DNA-binding domain of the hexameric arginine repressor. *Journal of Molecular Biology*, **1995**, 254, 150-62	6.5	54
195	Structural analysis of the two c(2 □2) phases of Na adsorbed on Al(100). *Surface Science*, **1995**, 330, 182-192	1.8	53
194	Theoretical analysis of the electronic structure of the stable and metastable c(2□2) phases of Na on Al(001): Comparison with angle-resolved ultraviolet photoemission spectra. *Physical Review B*, **1998**, 57, 15251-15260	3.3	52
193	Trends in adsorption of noble gases He, Ne, Ar, Kr, and Xe on Pd(111)(3□3)R30□: All-electron density-functional calculations. *Physical Review B*, **2008**, 77,	3.3	50
192	Low-energy electron-diffraction analysis of the (□ □)R19.1□-S adsorbate structure on the Pd(111) surface. *Surface Science*, **1994**, 317, 84-98	1.8	50
191	Magnetism of Co-doped ZnO epitaxially grown on a ZnO substrate. *Physical Review B*, **2012**, 85,	3.3	49
190	Evaluation of van der Waals density functionals for layered materials. *Physical Review Materials*, **2018**, 2,	3.2	47
189	Sensing sulfur-containing gases using titanium and tin decorated zigzag graphene nanoribbons from first-principles. *Physical Chemistry Chemical Physics*, **2015**, 17, 6925-32	3.6	46
188	Shape and surface structure of gold nanoparticles under oxidizing conditions. *Physical Review B*, **2008**, 77,	3.3	46
187	Formation and structural analysis of a surface alloy: Al(111)-(2 x 2)-Na. *Physical Review Letters*, **1995**, 74, 1617-1620	7.4	46
186	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	3.6	45

185	Surface properties of the refractory metal-nitride semiconductor ScN: Screened-exchange LDA-FLAPW investigations. *Physical Review B*, **2002**, 65,	3.3	44
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183	Stability, structure, and electronic properties of chemisorbed oxygen and thin surface oxides on Ir(111). *Physical Review B*, **2008**, 78,	3.3	42
182	Neutral and charged embedded clusters of Mn in doped GaN from first principles. *Physical Review B* , **2007**, 76,	3.3	41
181	Nitrogen vacancies in InN: Vacancy clustering and metallic bonding from first principles. *Physical Review B*, **2008**, 77,	3.3	40
180	First-principles investigation of Ag-Cu alloy surfaces in an oxidizing environment. *Physical Review B*, **2008**, 77,	3.3	40
179	Ab initio lattice dynamics and thermal expansion of Cu2O. *Physical Review B*, **2009**, 80,	3.3	39
178	Nitrogen adsorption and thin surface nitrides on Cu(111) from first-principles. *Surface Science*, **2007** , 601, 4775-4785	1.8	38
177	Half-metallicity and efficient spin injection in AlN/GaN:Cr (0001) heterostructure. *Physical Review Letters*, **2005**, 94, 146602	7.4	38
176	Embedded clustering in Cr-doped AlN: Evidence for general behavior in dilute magnetic III-nitride semiconductors. *Journal of Applied Physics*, **2007**, 101, 103917	2.5	37
175	First principles study of 3d transition metal doped . *Journal of Magnetism and Magnetic Materials*, **2012**, 324, 3138-3143	2.8	36
174	Morphology of copper nanoparticles in a nitrogen atmosphere: A first-principles investigation. *Physical Review B*, **2008**, 77,	3.3	36
173	Energy barriers and chemical properties in the coadsorption of carbon monoxide and oxygen on Ru(0001). *Physical Review B*, **2002**, 65,	3.3	36
172	Cooperation of Ni and CaO at Interface for CO2 Reforming of CH4: A Combined Theoretical and Experimental Study. *ACS Catalysis*, **2019**, 9, 10060-10069	13.1	35
171	Magic numbers of nanoholes in graphene: Tunable magnetism and semiconductivity. *Physical Review B*, **2011**, 84,	3.3	35
170	Band gap engineering of wurtzite and zinc-blende GaN/AlN superlattices from first principles. *Journal of Applied Physics*, **2010**, 108, 103701	2.5	35
169	Ag□u alloy surfaces in an oxidizing environment: A first-principles study. *Surface Science*, **2009**, 603, 1467-1475	1.8	35
168	Spatial distribution and magnetism in poly-Cr-doped GaN from first principles. *Physical Review B*, **2007**, 75,	3.3	35

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166	Hybrid functional calculations of point defects and hydrogen in SrZrO3. *Physical Review B*, **2014**, 89,	3.3	34
165	Theory of Adsorption on Metal Substrates. *Handbook of Surface Science*, **2000**, 285-356		34
164	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	3.5	34
163	Exploiting the Novel Electronic and Magnetic Structure of C3N via Functionalization and Conformation. *Advanced Electronic Materials*, **2019**, 5, 1900459	6.4	33
162	Multiple CO2 capture in stable metal-doped graphene: a theoretical trend study. *RSC Advances*, **2015**, 5, 50975-50982	3.7	33
161	Built-in electric fields and valence band offsets in InN/GaN(0001) superlattices: First-principles investigations. *Journal of Applied Physics*, **2011**, 109, 083721	2.5	33
160	Defect complexes and cluster doping of InN: First-principles investigations. *Physical Review B*, **2009**, 79,	3.3	33
159	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	6.7	32
158	Vacancies and interstitials in indium nitride: Vacancy clustering and molecular bondlike formation from first principles. *Physical Review B*, **2009**, 79,	3.3	32
157	Control of CN and CN carbon nitride nanosheetsNelectronic and magnetic properties through embedded atoms. *Physical Chemistry Chemical Physics*, **2020**, 22, 2249-2261	3.6	32
156	A Dirac-semimetal two-dimensional BeN4: Thickness-dependent electronic and optical properties. *Applied Physics Letters*, **2021**, 118, 203103	3.4	32
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154	A First-Principles Study of C N Nanostructures: Control and Engineering of the Electronic and Magnetic Properties of Nanosheets, Tubes and Ribbons. *ChemPhysChem*, **2020**, 21, 164-174	3.2	30
153	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	1.3	28
152	Cu/ZnO(0001) under oxidating and reducing conditions: A first-principles survey of surface structures. *Physical Review B*, **2011**, 84,	3.3	28
151	Atomic and electronic structure of single and multiple vacancies in GaN nanowires from first-principles. *Physical Review B*, **2009**, 79,	3.3	28
150	Reaction intermediates of methanol synthesis and the water–gas-shift reaction on the ZnO(0001) surface. *Surface Science*, **2010**, 604, 1742-1751	1.8	28

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148	Embedding of atoms into the nanopore sites of the CN and CN porous carbon nitride monolayers with tunable electronic properties. *Physical Chemistry Chemical Physics*, **2020**, 22, 6418-6433	3.6	27
147	Oxygen adsorption on the (1 1) and (2 1) reconstructed C(111) surfaces: a density functional theory study. *Journal of Physics Condensed Matter*, **2010**, 22, 265007	1.8	27
146	THEORETICAL EVIDENCE FOR UNUSUAL BONDING GEOMETRY AND PHASE TRANSITIONS OF Na ON Al(001). *Surface Review and Letters*, **1994**, 01, 213-219	1.1	27
145	Band-gap control of graphenelike borocarbonitride gBC6N bilayers by electrical gating. *Physical Review B*, **2020**, 102,	3.3	26
144	Dirac half-metallicity of Thin PdCl Nanosheets: Investigation of the Effects of External Fields, Surface Adsorption and Defect Engineering on the Electronic and Magnetic Properties. *Scientific Reports*, **2020**, 10, 213	4.9	26
143	Multiferroic crossover in perovskite oxides. *Physical Review B*, **2016**, 93,	3.3	26
142	Real Time Determination of the Electronic Structure of Unstable Reaction Intermediates during Au2O3 Reduction. *Journal of Physical Chemistry Letters*, **2014**, 5, 80-4	6.4	26
141	Playing with dimensions: rational design for heteroepitaxial p-n junctions. *Nano Letters*, **2012**, 12, 68-76	11.5	26
140	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	3.9	25
139	Density-functional prediction of a surface magnetic phase in SrTiO(3)/LaAlO(3) heterostructures induced by Al vacancies. *Physical Review Letters*, **2014**, 113, 186401	7.4	25
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137	A first-principles density functional study of chlorophenol adsorption on Cu2O(110):CuO. *Journal of Chemical Physics*, **2009**, 130, 184505	3.9	25
136	Nature of Xenon adsorption on graphite: On-top versus hollow site preference. *Physical Review B*, **2007**, 76,	3.3	25
135	Design of shallow acceptors in ZnO through early transition metals codoped with N acceptors. *Physical Review B*, **2011**, 83,	3.3	24
134	Mitigation of CO poisoning on functionalized Pt-TiN surfaces. *Physical Chemistry Chemical Physics*, **2013**, 15, 19450-6	3.6	23
133	Hydrogen Adsorption on Nearly Zigzag-Edged Nanoribbons: A Density Functional Theory Study. *Scientific Reports*, **2017**, 7, 15727	4.9	23
132	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, 155103	2.5	23

131	Acidity enhanced [Al]MCM-41 via ultrasonic irradiation for the Beckmann rearrangement of cyclohexanone oxime to e-caprolactam. *Journal of Catalysis*, **2018**, 358, 71-79	7.3	23
130	Unravelling the effects of layered supports on Ru nanoparticles for enhancing N2 reduction in photocatalytic ammonia synthesis. *Applied Catalysis B: Environmental*, **2019**, 259, 118026	21.8	22
129	Continuously tunable band gap in GaN/AlN (0001) superlattices via built-in electric field. *Physical Review B*, **2010**, 81,	3.3	22
128	Bridging the temperature and pressure gaps: close-packed transition metal surfaces in an oxygen environment. *Journal of Physics Condensed Matter*, **2008**, 20, 184021	1.8	22
127	Phase diagram of O/Ru(0001) from first principles. *Chemical Physics Letters*, **2002**, 361, 317-320	2.5	21
126	Machine learning the band gap properties of kesterite I2□II-IV-V4 quaternary compounds for photovoltaics applications. *Physical Review Materials*, **2018**, 2,	3.2	21
125	First-principles study of the mechanism of ethylene epoxidation over Ag□u particles. *Journal of Materials Chemistry*, **2010**, 20, 10521		20
124	Doping of AlGaN Alloys. *MRS Internet Journal of Nitride Semiconductor Research*, **1999**, 4, 890-901		20
123	Defects and Defect Reactions in Semiconductor Nitrides. *Acta Physica Polonica A*, **1999**, 96, 613-627	0.6	20
122	A new LEED investigation of the Cu(110)-(2 □)N structure. *Surface Science*, **1997**, 381, L589-L593	1.8	19
121	The structure ofAl(111)-K(□ □)R30°determined by LEED: stable and metastable adsorption sites. *Surface Science*, **1993**, 287-288, 418-422	1.8	19
120	Strongly enhanced acidity and activity of amorphous silica□lumina by formation of pentacoordinated AlV species. *Journal of Catalysis*, **2019**, 372, 1-7	7.3	19
119	Structural and electronic properties of SrZrO3 and Sr(Ti,Zr)O3 alloys. *Physical Review B*, **2015**, 92,	3.3	18
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117	Density of configurational states from first-principles calculations: the phase diagram of Al-Na surface alloys. *ChemPhysChem*, **2005**, 6, 1923-8	3.2	18
116	Boron-Doped g-C6N6 Layer as a Metal-Free Photoelectrocatalyst for N2 Reduction Reaction. *Journal of Physical Chemistry C*, **2019**, 123, 28739-28743	3.8	17
115	Comparison of hydrogen and deuterium adsorption on Pd(100). *Journal of Chemical Physics*, **2010**, 132, 024714	3.9	17
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111	Bistable Magnetism and Potential for Voltage-Induced Spin Crossover in Dilute Magnetic Ferroelectrics. *Physical Review Letters*, **2015**, 114, 247601	7.4	15
110	Microscopic origin of n-type behavior in Si-doped AlN. *Physical Review B*, **2013**, 88,	3.3	15
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108	Magnetoresistivity model and ionization-energy approximation for ferromagnets. *Physica Status Solidi (B): Basic Research*, **2009**, 246, 1060-1071	1.3	15
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103	Challenges in predictive calculations of processes at surfaces:. surface thermodynamics and catalytic reactions. *Applied Physics A: Materials Science and Processing*, **1999**, 69, 471-480	2.6	14
102	Tunable electronic properties of the dynamically stable layered mineral PtHgSe (Jacutingaite). *Physical Chemistry Chemical Physics*, **2020**, 22, 24471-24479	3.6	14
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100	Acceptor doping in the proton conductor SrZrO. *Physical Chemistry Chemical Physics*, **2017**, 19, 11485-11491	3.6	13
99	CHx adsorption (x = 1-4) and thermodynamic stability on the CeO2(111) surface: a first-principles investigation. *RSC Advances*, **2014**, 4, 12245	3.7	13
98	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	3.8	13
97	Band offsets and polarization effects in wurtzite ZnO/Mg0.25Zn0.75O superlattices from first principles. *Physical Review B*, **2012**, 86,	3.3	13
96	Coverage and charge-state dependent adsorption of carbon monoxide on the zinc oxide (0001) surface. *Physical Review B*, **2010**, 82,	3.3	13

95	Quantum confinement effects in gallium nitride nanostructures: ab initio investigations. *Nanotechnology*, **2009**, 20, 425401	3.4	13
94	First-principles design of bifunctional oxygen reduction and evolution catalysts through bimetallic centers in metal□rganic frameworks. *Catalysis Science and Technology*, **2018**, 8, 3666-3674	5.5	13
93	High On/Off Conductance Switching Ratio via H-Tautomerization in Quinone. *Journal of Chemical Theory and Computation*, **2015**, 11, 4154-8	6.4	12
92	Identification of Vicinal Silanols and Promotion of Their Formation on MCM-41 via Ultrasonic Assisted One-Step Room-Temperature Synthesis for Beckmann Rearrangement. *Industrial & Engineering Chemistry Research*, **2018**, 57, 5550-5557	3.9	12
91	Built-in electric field assisted spin injection in Cr and Mn □layer doped AlN/GaN(0001) heterostructures from first principles. *Physical Review B*, **2008**, 78,	3.3	12
90	Strain-Engineered Ultrahigh Mobility in Phosphorene for Terahertz Transistors. *Advanced Electronic Materials*, **2019**, 5, 1800797	6.4	12
89	Magnetic properties of stoichiometric and defective CoS. *Physical Chemistry Chemical Physics*, **2018**, 20, 2356-2362	3.6	11
88	Catalytic arene alkylation over H-Beta zeolite: Influence of zeolite shape selectivity and reactant nucleophilicity. *Journal of Catalysis*, **2019**, 380, 9-20	7.3	11
87	Mechanism of efficient carbon monoxide oxidation at Ru(0001). *Journal of Vacuum Science and Technology A: Vacuum, Surfaces and Films*, **1997**, 15, 1635-1641	2.9	11
86	Resolving Deactivation Pathways of Co Porphyrin-Based Electrocatalysts for CO2 Reduction in Aqueous Medium. *ACS Catalysis*, **2021**, 11, 3715-3729	13.1	11
85	Composition-structure-function correlation of Ca/Zn/AlOx catalysts for the ketonization of acetic acid. *Catalysis Today*, **2020**, 351, 58-67	5.3	11
84	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	3.8	11
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