BjÃ¸rk Hammer

List of Publications by Year
in descending order

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230	44,502	5876 81	1895 208
papers	citations	h-index	g-index

239	239	239	30136
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	Improved adsorption energetics within density-functional theory using revised Perdew-Burke-Ernzerhof functionals. Physical Review B, 1999, 59, 7413-7421.	1.1	6,206
2	Why gold is the noblest of all the metals. Nature, 1995, 376, 238-240.	13.7	2,902
3	Electronic factors determining the reactivity of metal surfaces. Surface Science, 1995, 343, 211-220.	0.8	2,087
4	Effect of Strain on the Reactivity of Metal Surfaces. Physical Review Letters, 1998, 81, 2819-2822.	2.9	2,001
5	The atomic simulation environmentâ€”a Python library for working with atoms. Journal of Physics Condensed Matter, 2017, 29, 273002.	0.7	1,933
6	Theoretical surface science and catalysisâ€”calculations and concepts. Advances in Catalysis, 2000, 45, 71-129.	0.1	1,776
7	Electronic structure calculations with GPAW: a real-space implementation of the projector augmented-wave method. Journal of Physics Condensed Matter, 2010, 22, 253202.	0.7	1,451
8	Bandgap opening in graphene induced by patterned hydrogen adsorption. Nature Materials, 2010, 9, 315-319.	13.3	1,344
9	CO Chemisorption at Metal Surfaces and Overlayers. Physical Review Letters, 1996, 76, 2141-2144.	2.9	1,293
10	Universality in Heterogeneous Catalysis. Journal of Catalysis, 2002, 209, 275-278.	3.1	1,167
11	Surface electronic structure and reactivity of transition and noble metals1Communication presented at the First Francqui Colloquium, Brussels, 19â€“20 February 1996.1. Journal of Molecular Catalysis A, 1997, 115, 421-429.	4.8	1,166
12	Design of a Surface Alloy Catalyst for Steam Reforming. Science, 1998, 279, 1913-1915.	6.0	951
13	The Role of Interstitial Sites in the Ti 3d Defect State in the Band Gap of Titania. Science, 2008, 320, 1755-1759.	6.0	813
14	The CO/Pt(111) Puzzle. Journal of Physical Chemistry B, 2001, 105, 4018-4025.	1.2	642
15	The BrÃ¸nstedâ€“Evansâ€“Polanyi Relation and the Volcano Plot for Ammonia Synthesis over Transition Metal Catalysts. Journal of Catalysis, 2001, 197, 229-231.	3.1	582
16	Chiral recognition in dimerization of adsorbed cysteine observed by scanning tunnelling microscopy. Nature, 2002, 415, 891-893.	13.7	569
17	Oxygen vacancies on TiO2(110) and their interaction with H2O and O2: A combined high-resolution STM and DFT study. Surface Science, 2005, 598, 226-245.	0.8	560
18	Enhanced Bonding of Gold Nanoparticles on Oxidized TiO2(110). Science, 2007, 315, 1692-1696.	6.0	459

#	Article	IF	Citations
19	Structure sensitivity in adsorption: CO interaction with stepped and reconstructed Pt surfaces. Catalysis Letters, 1997, 46, 31-35.	1.4	453
20	Active Role of Oxide Support during CO Oxidation atAu/MgO. Physical Review Letters, 2003, 90, 206102.	2.9	431
21	Formation and Splitting of Paired Hydroxyl Groups on ReducedTiO2(110). Physical Review Letters, 2006, 96, 066107.	2.9	389
22	The electronic structure effect in heterogeneous catalysis. Catalysis Letters, 2005, 100, 111-114.	1.4	349
23	Multidimensional Potential Energy Surface forH2Dissociation over Cu(111). Physical Review Letters, 1994, 73, 1400-1403.	2.9	334
24	Structure and Reactivity of Surface Oxides on Pt(110) during Catalytic CO Oxidation. Physical Review Letters, 2005, 95, 255505.	2.9	327
25	Metastable Structures and Recombination Pathways for Atomic Hydrogen on the Graphite (0001) Surface. Physical Review Letters, 2006, 96, 156104.	2.9	296
26	Adsorption of O2 and oxidation of CO at Au nanoparticles supported by TiO2(110). Journal of Chemical Physics, 2004, 120, 7673-7680.	1.2	294
27	Guanine Quartet Networks Stabilized by Cooperative Hydrogen Bonds. Angewandte Chemie - International Edition, 2005, 44, 2270-2275.	7.2	275
28	Special Sites at Noble and Late Transition Metal Catalysts. Topics in Catalysis, 2006, 37, 3-16.	1.3	274
29	A theoretical study of CH4 dissociation on pure and goldâ€alloyed Ni(111) surfaces. Journal of Chemical Physics, 1996, 105, 5595-5604.	1.2	262
30	Clustering of Chemisorbed H(D) Atoms on the Graphite (0001) Surface due to Preferential Sticking. Physical Review Letters, 2006, 97, 186102.	2.9	260
31	A density functional theory study of the adsorption of sulfur, mercapto, and methylthiolate on Au(111). Journal of Chemical Physics, 2002, 116, 784-790.	1.2	253
32	Adsorption, diffusion, and dissociation of molecular oxygen at defected TiO2(110): A density functional theory study. Journal of Chemical Physics, 2004, 120, 988-997.	1.2	251
33	Theoretical study of CO oxidation on Au nanoparticles supported by MgO(100). Physical Review B, 2004, 69, .	1.1	246
34	Selective Propene Epoxidation on Immobilized Au_{6â€“10} Clusters: The Effect of Hydrogen and Water on Activity and Selectivity. Angewandte Chemie - International Edition, 2009, 48, 1467-1471.	7.2	246
35	Some recent theoretical advances in the understanding of the catalytic activity of Au. Applied Catalysis A: General, 2005, 291, 21-31.	2.2	240
36	Chiral switching by spontaneous conformational change in adsorbed organic molecules. Nature Materials, 2006, 5, 112-117.	13.3	213

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37	Local Chemical Reactivity of a Metal Alloy Surface. Physical Review Letters, 1995, 74, 3487-3490.	2.9	210
38	Theoretical analysis of hydrogen chemisorption on Pd(111), Re(0001) andPdML/Re(0001),ReML/Pd(111)pseudomorphic overlayers. Physical Review B, 1999, 60, 6146-6154.	1.1	207
39	Covalent Interlinking of an Aldehyde and an Amine on a Au(111) Surface in Ultrahigh Vacuum. Angewandte Chemie - International Edition, 2007, 46, 9227-9230.	7.2	191
40	Oxygen Dissociation at Pt Steps. Physical Review Letters, 2001, 87, 056103.	2.9	189
41	Alkali Promotion ofN2Dissociation over Ru(0001). Physical Review Letters, 1998, 80, 4333-4336.	2.9	185
42	Bond Activation at Monatomic Steps: NO Dissociation at Corrugated Ru(0001). Physical Review Letters, 1999, 83, 3681-3684.	2.9	183
43	Role of nonlocal exchange correlation in activated adsorption. Physical Review Letters, 1993, 70, 3971-3974.	2.9	170
44	A genetic algorithm for first principles global structure optimization of supported nano structures. Journal of Chemical Physics, 2014, 141, 044711.	1.2	166
45	Theoretical study of thiol-induced reconstructions on the Au(111) surface. Chemical Physics Letters, 2002, 360, 264-271.	1.2	161
46	Nitrogen Adsorption and Dissociation on Fe(111). Journal of Catalysis, 1999, 182, 479-488.	3.1	150
47	Role ofAu+in Supporting and ActivatingAu7onTiO2(110). Physical Review Letters, 2006, 97, 136107.	2.9	149
48	Sulfur bonding in MoS2 and Co-Mo-S structures. Catalysis Letters, 1997, 47, 177-182.	1.4	146
49	The NO+CO Reaction Catalyzed by Flat, Stepped, and Edged Pd Surfaces. Journal of Catalysis, 2001, 199, 171-176.	3.1	146
50	High-Dimensional Quantum Dynamics of Adsorption and Desorption ofH2at Cu(111). Physical Review Letters, 1994, 73, 3121-3124.	2.9	145
51	In Situ Detection of Active Edge Sites in Single-Layer MoS₂ Catalysts. ACS Nano, 2015, 9, 9322-9330.	7.3	144
52	Adsorption, diffusion, and dissociation of NO, N and O on flat and stepped Ru(0001). Surface Science, 2000, 459, 323-348.	0.8	140
53	Dissociative and molecular oxygen chemisorption channels on reduced rutile TiO2(110): An STM and TPD study. Surface Science, 2010, 604, 1945-1960.	0.8	132
54	One-DimensionalPtO2at Pt Steps: Formation and Reaction with CO. Physical Review Letters, 2005, 95, 256102.	2.9	131

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55	Oxidation of Pt(110). Physical Review Letters, 2004, 93, 146104.	2.9	129
56	DFT + U study of defects in bulk rutile TiO2. Journal of Chemical Physics, 2010, 133, 144708.	1.2	126
57	The activity of the tetrahedral Au20 cluster: charging and impurity effects. Journal of Catalysis, 2005, 233, 399-404.	3.1	124
58	2Dâ”3D Transition for Cationic and Anionic Gold Clusters: A Kinetic Energy Density Functional Study. Journal of the American Chemical Society, 2009, 131, 10605-10609.	6.6	124
59	A theoretical study of adsorbateâ€“adsorbate interactions on Ru(0001). Surface Science, 1998, 414, 315-329.	0.8	123
60	Single-layer<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:msub><mml:mtext>MoS</mml:mtext><mml:mn>2</mml:mn></mml:msub> Au(111): Band gap renormalization and substrate interaction. Physical Review B, 2016, 93, .	1.1	123
61	Chiral Recognition of Organic Molecules by Atomic Kinks on Surfaces. Physical Review Letters, 2006, 96, 056103.	2.9	120
62	Systematic Study of<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:msub><mml:mi>Au</mml:mi><mml:mn>6</mml:mn></mml:msub></mml:math>to<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:msub><mml:mi>Au</mml:mi><mml:mn>12</mml:mn></mml:msub></mml:math>Gold Clusters on MgO(100)<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mi>F</mml:mi></mml:math>Centers Using Density-Functional Theory. Physical Re	2.9	120
63	Electronic structure, total energies, and STM images of clean and oxygen-covered Al(111). Physical Review B, 1995, 52, 14954-14962.	1.1	118
64	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.	0.8	114
65	Density Functional Calculations of N2Adsorption and Dissociation on a Ru(0001) Surface. Journal of Catalysis, 1997, 169, 85-92.	3.1	112
66	Growth of Unidirectional Molecular Rows of Cysteine onAu(110)â”(1Ã—2)Driven by Adsorbate-Induced Surface Rearrangements. Physical Review Letters, 2004, 93, 086101.	2.9	112
67	The dynamics of H absorption in and adsorption on Cu(111). Surface Science, 1998, 397, 382-394.	0.8	111
68	On-the-Fly Machine Learning of Atomic Potential in Density Functional Theory Structure Optimization. Physical Review Letters, 2018, 120, 026102.	2.9	104
69	Observation of All the Intermediate Steps of a Chemical Reaction on an Oxide Surface by Scanning Tunneling Microscopy. ACS Nano, 2009, 3, 517-526.	7.3	101
70	Geometric and electronic factors determining the differences in reactivity of H2 on Cu(100) and Cu(111). Surface Science, 1996, 359, 45-53.	0.8	100
71	Water Adsorption on TiO2. Topics in Catalysis, 2010, 53, 423-430.	1.3	100
72	Nitrogen adsorption on Fe(111), (100), and (110) surfaces. Surface Science, 1999, 422, 8-16.	0.8	97

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73	CO adsorption and dissociation on Pt(111) and Ni(111) surfaces. Surface Science, 1997, 386, 67-72.	0.8	91
74	Neural-network-enhanced evolutionary algorithm applied to supported metal nanoparticles. Physical Review B, 2018, 97, .	1.1	90
75	Formation and Diffusion of Water Dimers on Rutile<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:msub><mml:mi>TiO</mml:mi><mml:mn>2</mml:mn></mml:msub><mml:mo stretchy="false">(</mml:mo><mml:mn>110</mml:mn><mml:mo) Tj ETQq1 1 0.784314 rgBT /Overlock 10 Tf 50 647 Td (stretchy="fa	2.9	89
76	Graphene Coatings: Probing the Limits of the One Atom Thick Protection Layer. ACS Nano, 2012, 6, 10258-10266.	7.3	89
77	Efficient Global Structure Optimization with a Machine-Learned Surrogate Model. Physical Review Letters, 2020, 124, 086102.	2.9	87
78	Direct pathway for sticking/desorption ofH2on Si(100). Physical Review B, 1995, 51, 13432-13440.	1.1	84
79	Imaging of the Hydrogen Subsurface Site in Rutile<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:msub><mml:mi>TiO</mml:mi><mml:mn>2</mml:mn></mml:msub></mml:math>. Physical Review Letters, 2009, 102, 136103.	2.9	84
80	Direct Observation of Molecular Preorganization for Chirality Transfer on a Catalyst Surface. Science, 2011, 334, 776-780.	6.0	84
81	Dissociation path forH2on Al(110). Physical Review Letters, 1992, 69, 1971-1974.	2.9	80
82	Extended atomic hydrogen dimer configurations on the graphite(0001) surface. Journal of Chemical Physics, 2009, 131, 084706.	1.2	80
83	CO Intercalation of Graphene on Ir(111) in the Millibar Regime. Journal of Physical Chemistry C, 2013, 117, 16438-16447.	1.5	79
84	Designing surface alloys with specific active sites. Catalysis Letters, 1996, 40, 131-135.	1.4	77
85	Crystalline and electronic structure of single-layer<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:msub><mml:mi>TaS</mml:mi><mml:mn>2</mml:mn></mml:msub></mml:math>. Physical Review B, 2016, 94, .	1.1	77
86	Oxygen adsorption at anionic free and supported Au clusters. Journal of Chemical Physics, 2005, 123, 161104.	1.2	76
87	Oxidation state of oxide supported nanometric gold. Topics in Catalysis, 2007, 44, 49-56.	1.3	75
88	EXPERIMENTAL EVIDENCE FOR THE FORMATION OF HIGHLY SUPERHYDROGENATED POLYCYCLIC AROMATIC HYDROCARBONS THROUGH H ATOM ADDITION AND THEIR CATALYTIC ROLE IN H₂FORMATION. Astrophysical Journal, 2012, 752, 3.	1.6	75
89	Inverted vibrational distributions from N2 recombination at Ru(001): Evidence for a metastable molecular chemisorption well. Journal of Chemical Physics, 1999, 110, 6954-6962.	1.2	73
90	Adsorbate-Induced Alloy Phase Separation: A Direct View by High-Pressure Scanning Tunneling Microscopy. Physical Review Letters, 2005, 95, 126101.	2.9	72

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91	An automated nudged elastic band method. Journal of Chemical Physics, 2016, 145, 094107.	1.2	72
92	Structure and activity of oxidized Pt(110) and Î±-PtO2. Physical Chemistry Chemical Physics, 2006, 8, 1566.	1.3	71
93	Structure and catalytic reactivity of Rh oxides. Catalysis Today, 2009, 145, 227-235.	2.2	71
94	Visualizing hydrogen-induced reshaping and edge activation in MoS2 and Co-promoted MoS2 catalyst clusters. Nature Communications, 2018, 9, 2211.	5.8	71
95	Nitrogen Adsorption and Hydrogenation on aMoFe6S9Complex. Physical Review Letters, 1999, 82, 4054-4057.	2.9	70
96	Identification of the Catalytic Site at the Interface Perimeter of Au Clusters on Rutile TiO₂(110). ACS Catalysis, 2014, 4, 1626-1631.	5.5	70
97	Growth and electronic structure of epitaxial single-layer<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:msub><mml:mtext>WS</mml:mtext><mml:mn>2</mml:mn></mml:msub> Au(111). Physical Review B, 2015, 92, .	1.1	70
98	The mechanism of Mg²⁺ conduction in ammine magnesium borohydride promoted by a neutral molecule. Physical Chemistry Chemical Physics, 2020, 22, 9204-9209.	1.3	70
99	Comment on â€œHigh Pressure Adsorbate Structures Studied by Scanning Tunneling Microscopy: CO on Pt(111) in Equilibrium with the Gas Phaseâ€• Physical Review Letters, 2002, 88, 259601.	2.9	69
100	Controlling Hydrogenation of Graphene on Ir(111). ACS Nano, 2013, 7, 3823-3832.	7.3	69
101	Theory of Adsorption and Surface Reactions. , 1997, , 285-351.		69
102	Adsorbate Reorganization at Steps: NO on Pd(211). Physical Review Letters, 1997, 79, 4441-4444.	2.9	68
103	A first-principles potential energy surface for Eleyâ€“Rideal reaction dynamics of H atoms on Cu(111). Journal of Chemical Physics, 1999, 110, 2240-2249.	1.2	68
104	Coverage dependence ofN2dissociation at an N, O, or H precovered Ru(0001) surface investigated with density functional theory. Physical Review B, 2001, 63, .	1.1	67
105	Steps on rutile TiO<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>(110): Active sites for water and methanol dissociation. Physical Review B, 2011, 84, .	1.1	67
106	The coupling between adsorption dynamics and the surface structure: H2 on Si(100). Chemical Physics Letters, 1994, 229, 645-649.	1.2	65
107	Density Functional Theory Study of Enantiospecific Adsorption at Chiral Surfaces. Journal of the American Chemical Society, 2002, 124, 14789-14794.	6.6	64
108	Guanine Quartet Networks Stabilized by Cooperative Hydrogen Bonds. Angewandte Chemie, 2005, 117, 2310-2315.	1.6	64

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109	Reactivity of a stepped surface NO dissociation on Pd(211). Faraday Discussions, 1998, 110, 323-333.	1.6	63
110	Promoting and poisoning effects of Na and Cl coadsorption on CO oxidation over MgO-supported Au nanoparticles. Journal of Catalysis, 2004, 227, 217-226.	3.1	61
111	Role of Steps in the Dissociative Adsorption of Water on Rutile<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:msub><mml:mi>TiO</mml:mi><mml:mn>2</mml:mn></mml:msub><mml:mo stretchy="false">(</mml:mo><mml:mn>110</mml:mn><mml:mo) Tj ETQq1 1 0.784314 rgBT /Overlock 10 Tf 50 647 Td (stretchy="fa	2.9	61
112	A Surface Coordination Network Based on Copper Adatom Trimers. Angewandte Chemie - International Edition, 2014, 53, 12955-12959.	7.2	61
113	Probing Enantioselectivity with X-Ray Photoelectron Spectroscopy and Density Functional Theory. Physical Review Letters, 2007, 98, 136102.	2.9	58
114	Direct Evidence for Ethanol Dissociation on Rutile<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:msub><mml:mi>TiO</mml:mi><mml:mn>2</mml:mn></mml:msub><mml:mo stretchy="false">(</mml:mo><mml:mn>110</mml:mn><mml:mo) Tj ETQq0 0 0 rgBT /Overlock 10 Tf 50 527 Td (stretchy="false">)</mm	2.9	58
115	Graphene on metal surfaces and its hydrogen adsorption: A meta-GGA functional study. Physical Review B, 2012, 86, .	1.1	57
116	â€œErratum to Electronic factors determining the reactivity of metal surfacesâ€•[Surface Science 343 (1995) 211]. Surface Science, 1996, 359, 306.	0.8	56
117	Quantum-mechanical calculation of H on Ni(001) using a model potential based on first-principles calculations. Physical Review B, 1997, 56, 2258-2266.	1.1	56
118	Exploration versus Exploitation in Global Atomistic Structure Optimization. Journal of Physical Chemistry A, 2018, 122, 1504-1509.	1.1	56
119	Treatment of Layered Structures Using a Semilocal meta-GGA Density Functional. Journal of Physical Chemistry Letters, 2010, 1, 515-519.	2.1	55
120	Symmetry-Driven Band Gap Engineering in Hydrogen Functionalized Graphene. ACS Nano, 2016, 10, 10798-10807.	7.3	55
121	Stacking fault energies in aluminium. Journal of Physics Condensed Matter, 1992, 4, 10453-10460.	0.7	54
122	Atomic Energies from a Convolutional Neural Network. Journal of Chemical Theory and Computation, 2018, 14, 3933-3942.	2.3	54
123	The interaction of hydrogen with the (110) surface of NiAl. Surface Science, 1995, 331-333, 811-817.	0.8	53
124	Reactivity of a gas/metal/metal-oxide three-phase boundary: CO oxidation at the Pt(111)â€“c(4Ã—2)-2CO/Î±-PtO2 phase boundary. Chemical Physics Letters, 2005, 409, 1-7.	1.2	52
125	CO Desorption Rate Dependence on CO Partial Pressure over Platinum Fuel Cell Catalysts. Fuel Cells, 2004, 4, 309-319.	1.5	49
126	Guanine- and Potassium-Based Two-Dimensional Coordination Network Self-Assembled on Au(111). Journal of the American Chemical Society, 2010, 132, 15927-15929.	6.6	49

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127	The energetics and dynamics of H2 dissociation on Al(110). Surface Science, 1994, 304, 131-144.	0.8	48
128	Activation in Prochiral Reaction Assemblies on Pt(111). Journal of the American Chemical Society, 2008, 130, 5386-5387.	6.6	48
129	Structure and reactivity of a model catalyst alloy under realistic conditions. Journal of Physics Condensed Matter, 2008, 20, 184018.	0.7	47
130	Combining Evolutionary Algorithms with Clustering toward Rational Global Structure Optimization at the Atomic Scale. Journal of Chemical Theory and Computation, 2017, 13, 1486-1493.	2.3	47
131	Theoretical study of H2O dissociation and CO oxidation on Pt2Mo(111). Journal of Catalysis, 2006, 243, 192-198.	3.1	45
132	Interaction between Coronene and Graphite from Temperature-Programmed Desorption and DFT-vdW Calculations: Importance of Entropic Effects and Insights into Graphite Interlayer Binding. Journal of Physical Chemistry C, 2013, 117, 13520-13529.	1.5	45
133	Unravelling Site-Specific Photo-Reactions of Ethanol on Rutile TiO2(110). Scientific Reports, 2016, 6, 21990.	1.6	45
134	Chemisorption and vibration of hydrogen on Cu(111). Surface Science, 1993, 285, 27-30.	0.8	43
135	Adsorbate-Oxide Interactions during theNO+COReaction on MgO(100) Supported Pd Monolayer Films. Physical Review Letters, 2002, 89, 016102.	2.9	43
136	Study of Alkylthiolate Self-assembled Monolayers on Au(111) Using a Semilocal meta-GGA Density Functional. Journal of Physical Chemistry C, 2012, 116, 7374-7379.	1.5	43
137	A comparison of quantum and classical dynamics of H2 dissociation on Cu(111). Surface Science, 1996, 364, 219-234.	0.8	42
138	Kinetics of fast island decay on Ag(111). Physical Review B, 2001, 63, .	1.1	42
139	Effect of subsurface Ti-interstitials on the bonding of small gold clusters on rutile TiO2(110). Journal of Chemical Physics, 2009, 130, 044704.	1.2	42
140	Structure and stability of small H clusters on graphene. Physical Review B, 2011, 83, .	1.1	41
141	Reduced Step Edges on Rutile<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:msub><mml:mi>TiO</mml:mi><mml:mn>2</mml:mn></mml:msub><mml:mo stretchy="false">(</mml:mo><mml:mn>110</mml:mn><mml:mo) Tj ETQq1 1 0.784314 rgBT /Overlock 10 Tf 50 127 Td (stretchy="false and Reactive Sites for Ethanol Dissociation. Physical Review Letters, 2012, 109, 155501.	7.7	41
142	Adsorption and dehydrogenation of tetrahydroxybenzene on Cu(111). Chemical Communications, 2013, 49, 9308.	2.2	40
143	An STM and DFT study of the ordered structures of NO on Pd(). Surface Science, 2002, 496, 1-9.	0.8	39
144	Extended One-Dimensional Supramolecular Assembly on a Stepped Surface. Physical Review Letters, 2008, 100, 046103.	2.9	38

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145	Self-consistent meta-generalized gradient approximation study of adsorption of aromatic molecules on noble metal surfaces. Journal of Chemical Physics, 2011, 135, 084704.	1.2	38
146	Dynamics of High-Barrier Surface Reactions: Laser-Assisted Associative Desorption ofN2from Ru(0001). Physical Review Letters, 2000, 84, 4906-4909.	2.9	37
147	H2dissociation at defected Cu: Preference for reaction at vacancy and kink sites. Physical Review B, 2002, 65, .	1.1	37
148	Stereodirection of an Î±-Ketoester at Sub-molecular Sites on Chirally Modified Pt(111): Heterogeneous Asymmetric Catalysis. Journal of the American Chemical Society, 2013, 135, 9999-10002.	6.6	37
149	Sequential oxygen and alkali intercalation of epitaxial graphene on Ir(111): enhanced many-body effects and formation of pn -interfaces. 2D Materials, 2014, 1, 025002.	2.0	36
150	Understanding intercalation structures formed under graphene on Ir(111). Physical Review B, 2014, 90, .	1.1	36
151	Ethanol Diffusion on Rutile TiO₂(110) Mediated by H Adatoms. Journal of Physical Chemistry Letters, 2012, 3, 283-288.	2.1	35
152	Machine learning enhanced global optimization by clustering local environments to enable bundled atomic energies. Journal of Chemical Physics, 2018, 149, 134104.	1.2	35
153	Water Dissociation and Hydroxyl Ordering on Anatase <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:msub><mml:mrow><mml:mi>TiO</mml:mi></mml:mrow><mml:mrow><mml:mn>2</mml:mn></mml:mrow></mml:msub></mml:mrow></mml:math> stretchy="false">(</mml:mo><mml:mn>001</mml:mn><mml:mo) Tj ETQq1 1 0.784314 rgBT /Overlock 10 Tf 50 412 Td (stretchy="false		

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163	Remote Activation of Chemical Bonds in Heterogeneous Catalysis. ACS Catalysis, 2014, 4, 1182-1188.	5.5	28
164	A Comparison of N₂ and CO Adsorption on Ru(001). Zeitschrift Fur Physikalische Chemie, 1997, 198, 113-122.	1.4	27
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