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	Generating stable molecules using imitation and reinforcement learning. Machine Learning: Science and Technology, 2022, 3, 015008.	2.4	4
2	Water Chemistry beneath Graphene: Condensation of a Dense OHâ€“H₂O Phase under Graphene. Journal of Physical Chemistry C, 2022, 126, 4347-4354.	1.5	4
3	Structure of an Ultrathin Oxide on Pt₃Sn(111) Solved by Machine Learning Enhanced Global Optimization**. Angewandte Chemie, 2022, 134, .	1.6	3
4	Dimerization of dehydrogenated polycyclic aromatic hydrocarbons on graphene. Journal of Chemical Physics, 2022, 156, 134703.	1.2	3
5	Structure of an Ultrathin Oxide on Pt₃Sn(111) Solved by Machine Learning Enhanced Global Optimization**. Angewandte Chemie - International Edition, 2022, 61, .	7.2	15
6	Global optimization of atomic structure enhanced by machine learning. Physical Review B, 2022, 105, .	1.1	22
7	Atomistic global optimization X: A Python package for optimization of atomistic structures. Journal of Chemical Physics, 2022, 157, .	1.2	14
8	Size-dependent phase stability in transition metal dichalcogenide nanoparticles controlled by metal substrates. Nanoscale, 2021, 13, 10167-10180.	2.8	4
9	Gaussian representation for image recognition and reinforcement learning of atomistic structure. Journal of Chemical Physics, 2020, 153, 044107.	1.2	16
10	Atomistic structure learning algorithm with surrogate energy model relaxation. Physical Review B, 2020, 102, .	1.1	21
11	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
12	Efficient Global Structure Optimization with a Machine-Learned Surrogate Model. Physical Review Letters, 2020, 124, 086102.	2.9	87
13	Structure prediction of surface reconstructions by deep reinforcement learning. Journal of Physics Condensed Matter, 2020, 32, 404005.	0.7	16
14	<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mrow><mml:msub><mml:mi mathvariant="normal">NH</mml:mi><mml:mn>3</mml:mn></mml:msub></mml:mrow></mml:math> on anatase <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mrow><mml:msub><mml:mi>TiO</mml:mi><mml:mn>2</mml:mn></mml:msub></mml:mrow></mml:math>: Diffusion mechanisms and the effect of intermolecular repulsion. Physical Review Materials, 2020, 4, .	0.9	5
15	Atomistic structure learning. Journal of Chemical Physics, 2019, 151, .	1.2	26
16	Chemically-resolved determination of hydrogenated grapheneâ€“substrate interaction. Physical Chemistry Chemical Physics, 2019, 21, 13462-13466.	1.3	7
17	Constructing convex energy landscapes for atomistic structure optimization. Physical Review B, 2019, 100, .	1.1	8
18	Effects of Gas-Phase Conditions and Particle Size on the Properties of Cu(111)-Supported Zn_yO_x Particles Revealed by Global Optimization and Ab Initio Thermodynamics. Journal of Physical Chemistry C, 2019, 123, 30903-30916.	1.5	17

#	Article	IF	Citations
19	Rotation and diffusion of naphthalene on Pt(111). Journal of Chemical Physics, 2018, 148, 124703.	1.2	3
20	Exciting H₂ Molecules for Graphene Functionalization. ACS Nano, 2018, 12, 513-520.	7.3	24
21	On-the-Fly Machine Learning of Atomic Potential in Density Functional Theory Structure Optimization. Physical Review Letters, 2018, 120, 026102.	2.9	104
22	Exploration versus Exploitation in Global Atomistic Structure Optimization. Journal of Physical Chemistry A, 2018, 122, 1504-1509.	1.1	56
23	NH3 adsorption on anatase-TiO2(101). Journal of Chemical Physics, 2018, 148, 124704.	1.2	11
24	Tight-Binding Approximation-Enhanced Global Optimization. Journal of Chemical Theory and Computation, 2018, 14, 2797-2807.	2.3	31
25	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:mo stretchy="false">(</mml:mo><mml:mn>001</mml:mn><mml:mo) Tj ETQq1 1 0.784314 rgBT /Overlock 10 Tf 50 492 Td (stretchy="false		

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37	Influence of CHÂ·Â·Â·N Interaction in the Self-Assembly of an Oligo(isoquinolyne-ethynylyne) Molecule with Distinct Conformational States. Langmuir, 2017, 33, 10782-10791.	1.6	3
38	Structure of the <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:mrow><mml:msub><mml:mrow><mml:mi>SnO</mml:mi></mml:mrow><mml:mrow><mml:mn>2 stretchy="false">(</mml:mo><mml:mn>110</mml:mn><mml:mo) Tj ETQq0 0 0 rgBT /Overlock 10 Tf 50 707 Td (stretchy="false">)</mm stretchy="false">(</mml:mo><mml:mn>4</mml:mn><mml:mo>Ã—</mml:mo><mml:mn>1</mml:mn><mml:mo) Tj ETQq0 0 0 rgBT /Ov 0961	2.9	26
39	Supramolecular Corrals on Surfaces Resulting from Aromatic Interactions of Nonplanar Triazoles. ACS Nano, 2017, 11, 8302-8310.	7.3	4
40	Substrate-induced semiconductor-to-metal transition in monolayer <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:msub><mml:mi>WS</mml:mi><mml:mn>2</mml:mn></mml:msub></mml: Physical Review B, 2017, 96, .	1.1	33
41	The influence of coronene super-hydrogenation on the coronene-graphite interaction. Journal of Chemical Physics, 2016, 145, 174708.	1.2	11
42	Pyridine adsorption and diffusion on Pt(111) investigated with density functional theory. Journal of Chemical Physics, 2016, 144, 164112.	1.2	15
43	Structure and role of metal clusters in a metal-organic coordination network determined by density functional theory. Journal of Chemical Physics, 2016, 144, 084708.	1.2	5
44	An automated nudged elastic band method. Journal of Chemical Physics, 2016, 145, 094107.	1.2	72
45	Reduction of CO₂ with Water on Pt-Loaded Rutile TiO₂(110) Modeled with Density Functional Theory. Journal of Physical Chemistry C, 2016, 120, 9160-9164.	1.5	29
46	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: Physical Review B, 2016, 94, .	1.1	52
47	Band-gap engineering by Bi intercalation of graphene on Ir(111). Physical Review B, 2016, 93, .	1.1	30
48	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></mml: Au(111): Band gap renormalization and substrate interaction. Physical Review B, 2016, 93, .	1.1	128
49	Selection of conformational states in surface self-assembly for a molecule with eight possible pairs of surface enantiomers. Chemical Communications, 2016, 52, 14023-14026.	2.2	9
50	Symmetry-Driven Band Gap Engineering in Hydrogen Functionalized Graphene. ACS Nano, 2016, 10, 10798-10807.	7.3	55
51	Unravelling Site-Specific Photo-Reactions of Ethanol on Rutile TiO2(110). Scientific Reports, 2016, 6, 21990.	1.6	45
52	Effects of particle size and edge structure on the electronic structure, spectroscopic features, and chemical properties of Au(111)-supported MoS₂ nanoparticles. Faraday Discussions, 2016, 188, 323-343.	1.6	22
53	A comparative study of diastereomeric complexes formed by a prochiral substrate and three structurally analogous chiral molecules on Pt(111). Surface Science, 2016, 646, 13-18.	0.8	9
54	Selection of conformational states in self-assembled surface structures formed from an oligo(naphthyleneâ€“ethynylene) 3-bit binary switch. Journal of Chemical Physics, 2015, 142, 101922.	1.2	5

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55	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	10
56	In Situ Detection of Active Edge Sites in Single-Layer MoS₂ Catalysts. ACS Nano, 2015, 9, 9322-9330.	7.3	144
57	Isolating a Reaction Intermediate in the Hydrogenation of 2,2,2-Trifluoroacetophenone on Pt(111). Journal of Physical Chemistry C, 2015, 119, 7319-7326.	1.5	10
58	Single-chiral-catalytic-surface-sites: STM and DFT study of stereodirecting complexes formed between (R)-1-(1-naphthyl)ethylamine and ketopantolactone on Pt(111). Catalysis Science and Technology, 2015, 5, 743-753.	2.1	15
59	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
60	Nucleation and growth of Pt nanoparticles on reduced and oxidized rutile TiO2 (110). Journal of Chemical Physics, 2014, 141, 214702.	1.2	27
61	Hydrogen bond rotations as a uniform structural tool for analyzing protein architecture. Nature Communications, 2014, 5, 5803.	5.8	20
62	Understanding intercalation structures formed under graphene on Ir(111). Physical Review B, 2014, 90, .	1.1	36
63	Thermodynamic aspects of dehydrogenation reactions on noble metal surfaces. Journal of Chemical Physics, 2014, 141, 174705.	1.2	15
64	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
65	Modeling Methyl Chloride Photo Oxidation by Oxygen Species on TiO2(110). Topics in Catalysis, 2014, 57, 171-176.	1.3	6
66	Remote Activation of Chemical Bonds in Heterogeneous Catalysis. ACS Catalysis, 2014, 4, 1182-1188.	5.5	28
67	A genetic algorithm for first principles global structure optimization of supported nano structures. Journal of Chemical Physics, 2014, 141, 044711.	1.2	166
68	A Surface Coordination Network Based on Copper Adatom Trimers. Angewandte Chemie - International Edition, 2014, 53, 12955-12959.	7.2	61
69	Structure determination of chemisorbed chirality transfer complexes: Accelerated STM analysis and exchange-correlation functional sensitivity. Surface Science, 2014, 629, 48-56.	0.8	25
70	Walking-like diffusion of two-footed asymmetric aromatic adsorbates on Pt(111). Surface Science, 2014, 629, 123-131.	0.8	19
71	Ein Metallâ€organisches Netzwerk auf Basis von Cuâ€Adatomâ€Trimeren. Angewandte Chemie, 2014, 126, 13169-13173.	1.6	11
72	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 ETQq0 0 0 rgBT /Overlock 10 Tf 50 47 Td (stretchy="false">)</mml	2.9	61

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73	CO Intercalation of Graphene on Ir(111) in the Millibar Regime. Journal of Physical Chemistry C, 2013, 117, 16438-16447.	1.5	79
74	A density functional theory study of atomic steps on stoichiometric rutile TiO2(110). Journal of Chemical Physics, 2013, 139, 234704.	1.2	12
75	Breakdown of the Graphene Coating Effect under Sequential Exposure to O₂ and H₂S. Journal of Physical Chemistry Letters, 2013, 4, 3770-3774.	2.1	15
76	Adsorption and dehydrogenation of tetrahydroxybenzene on Cu(111). Chemical Communications, 2013, 49, 9308.	2.2	40
77	Controlling Hydrogenation of Graphene on Ir(111). ACS Nano, 2013, 7, 3823-3832.	7.3	69
78	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
79	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
80	Interfacial oxygen under TiO2 supported Au clusters revealed by a genetic algorithm search. Journal of Chemical Physics, 2013, 139, 204701.	1.2	15
81	Adsorption, mobility, and dimerization of benzaldehyde on Pt(111). Journal of Chemical Physics, 2012, 136, 174706.	1.2	20
82	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
83	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 50 327 Td (stretchy="false	2.9	41
84	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	2.9	120
85	Scanning Tunneling Microscopy Measurements of the Full Cycle of a Heterogeneous Asymmetric Hydrogenation Reaction on Chirally Modified Pt(111). Journal of Physical Chemistry Letters, 2012, 3, 92-96.	2.1	10
86	Ethanol Diffusion on Rutile TiO₂(110) Mediated by H Adatoms. Journal of Physical Chemistry Letters, 2012, 3, 283-288.	2.1	35
87	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
88	Preservation of the Pt(100) surface reconstruction after growth of a continuous layer of graphene. Surface Science, 2012, 606, 464-469.	0.8	22
89	Graphene on metal surfaces and its hydrogen adsorption: A meta-GGA functional study. Physical Review B, 2012, 86, .	1.1	57
90	Graphene Coatings: Probing the Limits of the One Atom Thick Protection Layer. ACS Nano, 2012, 6, 10258-10266.	7.3	89

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91	Packing Defects into Ordered Structures: Strands on<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, 2012, 108, 236103.	2.9	26
92	Linear hydrogen adsorbate structures on graphite induced by self-assembled molecular monolayers. Carbon, 2012, 50, 2052-2056.	5.4	12
93	Tuning Arylâ˜CHÂ·Â·Â·O Intermolecular Interactions on Pt(111). Journal of Physical Chemistry C, 2011, 115, 1355-1360.	1.5	17
94	Adsorption properties versus oxidation states of rutile TiO2(110). Journal of Chemical Physics, 2011, 134, 194703.	1.2	32
95	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 ETQq1 1 0.784314 rgBT /Overlock 10 Tf 50 567 Td (stretchy="false	2.9	58
96	Pyrene: Hydrogenation, hydrogen evolution, and Ï€-band model. Journal of Chemical Physics, 2011, 134, 164703.	1.2	32
97	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
98	Direct Observation of Molecular Preorganization for Chirality Transfer on a Catalyst Surface. Science, 2011, 334, 776-780.	6.0	84
99	Structure and stability of small H clusters on graphene. Physical Review B, 2011, 83, .	1.1	41
100	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
101	Water Adsorption on TiO2. Topics in Catalysis, 2010, 53, 423-430.	1.3	100
102	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
103	Alkane dimers interaction: A semi-local MGGA functional study. Chemical Physics Letters, 2010, 492, 183-186.	1.2	17
104	Bandgap opening in graphene induced by patterned hydrogen adsorption. Nature Materials, 2010, 9, 315-319.	13.3	1,344
105	EnevoldsenetÂal.Reply:. Physical Review Letters, 2010, 104, .	2.9	11
106	Comment on â€œOxygen Vacancy Origin of the Surface Band-Gap State of<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 50 132 Td (stretchy="false">)</mm	2.9	30
107	259704. CO oxidation on fully oxygen covered Ru(0001): Role of step edges. Physical Review B, 2010, 81, .	1.1	23
108	DFT + U study of defects in bulk rutile TiO2. Journal of Chemical Physics, 2010, 133, 144708.	1.2	126

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109	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
110	Enhanced Bonding of Silver Nanoparticles on Oxidized TiO₂(110). Journal of Physical Chemistry C, 2010, 114, 16964-16972.	1.5	23
111	Treatment of Layered Structures Using a Semilocal meta-GGA Density Functional. Journal of Physical Chemistry Letters, 2010, 1, 515-519.	2.1	55
112	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
113	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
114	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
115	Structure and catalytic reactivity of Rh oxides. Catalysis Today, 2009, 145, 227-235.	2.2	71
116	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 ETQq0 0 0 rgBT /Overlock 10 Tf 50 447 Td (stretchy="false">)</mm	2.9	89
117	Extended atomic hydrogen dimer configurations on the graphite(0001) surface. Journal of Chemical Physics, 2009, 131, 084706.	1.2	80
118	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
119	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
120	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
121	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
122	Activation in Prochiral Reaction Assemblies on Pt(111). Journal of the American Chemical Society, 2008, 130, 5386-5387.	6.6	48
123	Structure and reactivity of a model catalyst alloy under realistic conditions. Journal of Physics Condensed Matter, 2008, 20, 184018.	0.7	47
124	Extended One-Dimensional Supramolecular Assembly on a Stepped Surface. Physical Review Letters, 2008, 100, 046103.	2.9	38
125	Probing Enantioselectivity with X-Ray Photoelectron Spectroscopy and Density Functional Theory. Physical Review Letters, 2007, 98, 136102.	2.9	58
126	Enhanced Bonding of Gold Nanoparticles on Oxidized TiO2(110). Science, 2007, 315, 1692-1696.	6.0	459

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127	Role of Surface Elastic Relaxations in an O-Induced Nanopattern onPt(110)â^'(1Ã—2). Physical Review Letters, 2007, 98, 115501.	2.9	25
128	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
129	Oxidation state of oxide supported nanometric gold. Topics in Catalysis, 2007, 44, 49-56.	1.3	75
130	Metastable Structures and Recombination Pathways for Atomic Hydrogen on the Graphite (0001) Surface. Physical Review Letters, 2006, 96, 156104.	2.9	296
131	Clustering of Chemisorbed H(D) Atoms on the Graphite (0001) Surface due to Preferential Sticking. Physical Review Letters, 2006, 97, 186102.	2.9	260
132	Structure and activity of oxidized Pt(110) and Î±-PtO2. Physical Chemistry Chemical Physics, 2006, 8, 1566.	1.3	71
133	Role ofAu+in Supporting and ActivatingAu7onTiO2(110). Physical Review Letters, 2006, 97, 136107.	2.9	149
134	Chiral switching by spontaneous conformational change in adsorbed organic molecules. Nature Materials, 2006, 5, 112-117.	13.3	213
135	Special Sites at Noble and Late Transition Metal Catalysts. Topics in Catalysis, 2006, 37, 3-16.	1.3	274
136	The Role of the Chiral Modifier on the Enantioselective Hydrogenation of Methyl Pyruvate on Pt(111). Catalysis Letters, 2006, 106, 111-114.	1.4	14
137	Theoretical study of H2O dissociation and CO oxidation on Pt2Mo(111). Journal of Catalysis, 2006, 243, 192-198.	3.1	45
138	Formation and Splitting of Paired Hydroxyl Groups on ReducedTiO2(110). Physical Review Letters, 2006, 96, 066107.	2.9	389
139	Chiral Recognition of Organic Molecules by Atomic Kinks on Surfaces. Physical Review Letters, 2006, 96, 056103.	2.9	120
140	Density functional theory study of water dissociation in a double water bilayer with or without coadsorption of CO on Pt(111). Journal of Chemical Physics, 2006, 124, 184704.	1.2	21
141	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
142	One-DimensionalPtO2at Pt Steps: Formation and Reaction with CO. Physical Review Letters, 2005, 95, 256102.	2.9	131
143	The activity of the tetrahedral Au20 cluster: charging and impurity effects. Journal of Catalysis, 2005, 233, 399-404.	3.1	124
144	Guanine Quartet Networks Stabilized by Cooperative Hydrogen Bonds. Angewandte Chemie - International Edition, 2005, 44, 2270-2275.	7.2	275

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145	Guanine Quartet Networks Stabilized by Cooperative Hydrogen Bonds. Angewandte Chemie, 2005, 117, 2310-2315.	1.6	64
146	Some Recent Theoretical Advances in the Understanding of the Catalytic Activity of Au. ChemInform, 2005, 36, no.	0.1	0
147	Some recent theoretical advances in the understanding of the catalytic activity of Au. Applied Catalysis A: General, 2005, 291, 21-31.	2.2	240
148	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
149	The electronic structure effect in heterogeneous catalysis. Catalysis Letters, 2005, 100, 111-114.	1.4	349
150	Adsorbate-Induced Alloy Phase Separation: A Direct View by High-Pressure Scanning Tunneling Microscopy. Physical Review Letters, 2005, 95, 126101.	2.9	72
151	Structure and Reactivity of Surface Oxides on Pt(110) during Catalytic CO Oxidation. Physical Review Letters, 2005, 95, 255505.	2.9	327
152	Oxygen adsorption at anionic free and supported Au clusters. Journal of Chemical Physics, 2005, 123, 161104.	1.2	76
153	Two-Step Reaction on a Strained, Nanoscale Segmented Surface. Physical Review Letters, 2004, 93, 126104.	2.9	28
154	Oxidation of Pt(110). Physical Review Letters, 2004, 93, 146104.	2.9	129
155	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
156	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
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