Bjrk Hammer

List of Publications by Citations

226 papers	37,305 citations	77 h-index	192 g-index
239 ext. papers	40,521 ext. citations	6.7 avg, IF	7.31 L-index

#	Paper	IF	Citations
226	Improved adsorption energetics within density-functional theory using revised Perdew-Burke-Ernzerhof functionals. *Physical Review B*, **1999**, 59, 7413-7421	3.3	5077
225	Why gold is the noblest of all the metals. *Nature*, **1995**, 376, 238-240	50.4	2251
224	Effect of Strain on the Reactivity of Metal Surfaces. *Physical Review Letters*, **1998**, 81, 2819-2822	7.4	1680
223	Electronic factors determining the reactivity of metal surfaces. *Surface Science*, **1995**, 343, 211-220	1.8	1679
222	Theoretical surface science and catalysis□alculations and concepts. *Advances in Catalysis*, **2000**, 45, 71-129	2.4	1332
221	Bandgap opening in graphene induced by patterned hydrogen adsorption. *Nature Materials*, **2010**, 9, 315-9	27	1229
220	CO chemisorption at metal surfaces and overlayers. *Physical Review Letters*, **1996**, 76, 2141-2144	7.4	1135
219	The atomic simulation environment-a Python library for working with atoms. *Journal of Physics Condensed Matter*, **2017**, 29, 273002	1.8	1097
218	Electronic structure calculations with GPAW: a real-space implementation of the projector augmented-wave method. *Journal of Physics Condensed Matter*, **2010**, 22, 253202	1.8	1092
217	Universality in Heterogeneous Catalysis. *Journal of Catalysis*, **2002**, 209, 275-278	7.3	1007
216	Surface electronic structure and reactivity of transition and noble metals1Communication presented at the First Francqui Colloquium, Brussels, 19□0 February 1996.1. *Journal of Molecular Catalysis A*, **1997**, 115, 421-429		1000
215	Design of a surface alloy catalyst for steam reforming. *Science*, **1998**, 279, 1913-5	33.3	852
214	The role of interstitial sites in the Ti3d defect state in the band gap of titania. *Science*, **2008**, 320, 1755-9	33.3	744
213	The CO/Pt(111) Puzzle. *Journal of Physical Chemistry B*, **2001**, 105, 4018-4025	3.4	579
212	Chiral recognition in dimerization of adsorbed cysteine observed by scanning tunnelling microscopy. *Nature*, **2002**, 415, 891-3	50.4	529
211	Oxygen vacancies on TiO2(1 1 0) and their interaction with H2O and O2: A combined high-resolution STM and DFT study. *Surface Science*, **2005**, 598, 226-245	1.8	511
210	The Br□sted□Evans□Polanyi Relation and the Volcano Plot for Ammonia Synthesis over Transition Metal Catalysts. *Journal of Catalysis*, **2001**, 197, 229-231	7.3	471

209	Enhanced bonding of gold nanoparticles on oxidized TiO2(110). *Science*, **2007**, 315, 1692-6	33.3	432
208	Active role of oxide support during CO oxidation at Au/MgO. *Physical Review Letters*, **2003**, 90, 206102	7.4	393
207	Structure sensitivity in adsorption: CO interaction with stepped and reconstructed Pt surfaces. *Catalysis Letters*, **1997**, 46, 31-35	2.8	382
206	Formation and splitting of paired hydroxyl groups on reduced TiO2(110). *Physical Review Letters*, **2006**, 96, 066107	7.4	362
205	Multidimensional potential energy surface for H2 dissociation over Cu(111). *Physical Review Letters*, **1994**, 73, 1400-1403	7.4	313
204	Structure and reactivity of surface oxides on Pt(110) during catalytic CO oxidation. *Physical Review Letters*, **2005**, 95, 255505	7.4	305
203	Metastable structures and recombination pathways for atomic hydrogen on the graphite (0001) surface. *Physical Review Letters*, **2006**, 96, 156104	7.4	278
202	Adsorption of O2 and oxidation of CO at Au nanoparticles supported by TiO2(110). *Journal of Chemical Physics*, **2004**, 120, 7673-80	3.9	271
201	Guanine quartet networks stabilized by cooperative hydrogen bonds. *Angewandte Chemie - International Edition*, **2005**, 44, 2270-5	16.4	262
200	The electronic structure effect in heterogeneous catalysis. *Catalysis Letters*, **2005**, 100, 111-114	2.8	253
199	A density functional theory study of the adsorption of sulfur, mercapto, and methylthiolate on Au(111). *Journal of Chemical Physics*, **2002**, 116, 784-790	3.9	241
198	Clustering of chemisorbed H(D) atoms on the graphite (0001) surface due to preferential sticking. *Physical Review Letters*, **2006**, 97, 186102	7.4	235
197	Special Sites at Noble and Late Transition Metal Catalysts. *Topics in Catalysis*, **2006**, 37, 3-16	2.3	235
196	Adsorption, diffusion, and dissociation of molecular oxygen at defected TiO2(110): a density functional theory study. *Journal of Chemical Physics*, **2004**, 120, 988-97	3.9	235
195	A theoretical study of CH4 dissociation on pure and gold-alloyed Ni(111) surfaces. *Journal of Chemical Physics*, **1996**, 105, 5595-5604	3.9	234
194	Theoretical study of CO oxidation on Au nanoparticles supported by MgO(100). *Physical Review B*, **2004**, 69,	3.3	230
193	Selective propene epoxidation on immobilized au(6-10) clusters: the effect of hydrogen and water on activity and selectivity. *Angewandte Chemie - International Edition*, **2009**, 48, 1467-71	16.4	224
192	Some recent theoretical advances in the understanding of the catalytic activity of Au. *Applied Catalysis A: General*, **2005**, 291, 21-31	5.1	222

191	Chiral switching by spontaneous conformational change in adsorbed organic molecules. *Nature Materials*, **2006**, 5, 112-7	27	196
190	Theoretical analysis of hydrogen chemisorption on Pd(111), Re(0001) and PdML/Re(0001), ReML/Pd(111) pseudomorphic overlayers. *Physical Review B*, **1999**, 60, 6146-6154	3.3	183
189	Covalent interlinking of an aldehyde and an amine on a Au(111) surface in ultrahigh vacuum. *Angewandte Chemie - International Edition*, **2007**, 46, 9227-30	16.4	180
188	Local Chemical Reactivity of a Metal Alloy Surface. *Physical Review Letters*, **1995**, 74, 3487-3490	7.4	179
187	Oxygen dissociation at Pt steps. *Physical Review Letters*, **2001**, 87, 056103	7.4	178
186	Bond Activation at Monatomic Steps: NO Dissociation at Corrugated Ru(0001). *Physical Review Letters*, **1999**, 83, 3681-3684	7.4	168
185	Alkali Promotion of N2 Dissociation over Ru(0001). *Physical Review Letters*, **1998**, 80, 4333-4336	7.4	158
184	Theoretical study of thiol-induced reconstructions on the Au(111) surface. *Chemical Physics Letters*, **2002**, 360, 264-271	2.5	155
183	Role of nonlocal exchange correlation in activated adsorption. *Physical Review Letters*, **1993**, 70, 3971-3974	7.4	155
182	Role of Au(+) in supporting and activating Au(7) on TiO(2)(110). *Physical Review Letters*, **2006**, 97, 136107	7.4	142
181	Nitrogen Adsorption and Dissociation on Fe(111). *Journal of Catalysis*, **1999**, 182, 479-488	7.3	133
180	High-dimensional quantum dynamics of adsorption and desorption of H2 at Cu(111). *Physical Review Letters*, **1994**, 73, 3121-3124	7.4	131
179	Adsorption, diffusion, and dissociation of NO, N and O on flat and stepped Ru(0001). *Surface Science*, **2000**, 459, 323-348	1.8	129
178	The NO+CO Reaction Catalyzed by Flat, Stepped, and Edged Pd Surfaces. *Journal of Catalysis*, **2001**, 199, 171-176	7.3	125
177	A genetic algorithm for first principles global structure optimization of supported nano structures. *Journal of Chemical Physics*, **2014**, 141, 044711	3.9	122
176	Oxidation of Pt(110). *Physical Review Letters*, **2004**, 93, 146104	7.4	122
175	One-dimensional PtO2 at Pt steps: formation and reaction with CO. *Physical Review Letters*, **2005**, 95, 256102	7.4	122
174	The activity of the tetrahedral Au20 cluster: charging and impurity effects. *Journal of Catalysis*, **2005**, 233, 399-404	7.3	122

173	Sulfur bonding in MoS2 and Co-Mo-S structures. *Catalysis Letters*, **1997**, 47, 177-182	2.8	120
172	2D-3D transition for cationic and anionic gold clusters: a kinetic energy density functional study. *Journal of the American Chemical Society*, **2009**, 131, 10605-9	16.4	119
171	In Situ Detection of Active Edge Sites in Single-Layer MoS2 Catalysts. *ACS Nano*, **2015**, 9, 9322-30	16.7	116
170	Dissociative and molecular oxygen chemisorption channels on reduced rutile TiO2(110): An STM and TPD study. *Surface Science*, **2010**, 604, 1945-1960	1.8	116
169	DFT+U study of defects in bulk rutile TiO(2). *Journal of Chemical Physics*, **2010**, 133, 144708	3.9	114
168	Electronic structure, total energies, and STM images of clean and oxygen-covered Al(111). *Physical Review B*, **1995**, 52, 14954-14962	3.3	110
167	A theoretical study of adsorbate□adsorbate interactions on Ru(0001). *Surface Science*, **1998**, 414, 315-329	1.8	109
166	Chiral recognition of organic molecules by atomic kinks on surfaces. *Physical Review Letters*, **2006**, 96, 056103	7.4	109
165	Growth of unidirectional molecular rows of cysteine on Au(110)-(1 x 2) driven by adsorbate-induced surface rearrangements. *Physical Review Letters*, **2004**, 93, 086101	7.4	109
164	Oxygen dissociation at close-packed Pt terraces, Pt steps, and Ag-covered Pt steps studied with density functional theory. *Surface Science*, **2002**, 515, 235-244	1.8	107
163	Systematic study of Au6 to Au12 gold clusters on MgO(100) F centers using density-functional theory. *Physical Review Letters*, **2012**, 108, 126101	7.4	103
162	The dynamics of H absorption in and adsorption on Cu(111). *Surface Science*, **1998**, 397, 382-394	1.8	103
161	Density Functional Calculations of N2Adsorption and Dissociation on a Ru(0001) Surface. *Journal of Catalysis*, **1997**, 169, 85-92	7.3	97
160	Single-layer MoS2 on Au(111): Band gap renormalization and substrate interaction. *Physical Review B*, **2016**, 93,	3.3	93
159	Observation of all the intermediate steps of a chemical reaction on an oxide surface by scanning tunneling microscopy. *ACS Nano*, **2009**, 3, 517-26	16.7	92
158	Water Adsorption on TiO2. *Topics in Catalysis*, **2010**, 53, 423-430	2.3	91
157	Nitrogen adsorption on Fe(111), (100), and (110) surfaces. *Surface Science*, **1999**, 422, 8-16	1.8	88
156	Geometric and electronic factors determining the differences in reactivity of H2 on Cu(100) and Cu(111). *Surface Science*, **1996**, 359, 45-53	1.8	88

155	CO adsorption and dissociation on Pt(111) and Ni(111) surfaces. *Surface Science*, **1997**, 386, 67-72	1.8	85
154	Direct pathway for sticking/desorption of H2 on Si(100). *Physical Review B*, **1995**, 51, 13432-13440	3.3	82
153	Graphene coatings: probing the limits of the one atom thick protection layer. *ACS Nano*, **2012**, 6, 10258-66	13.7	81
152	Direct observation of molecular preorganization for chirality transfer on a catalyst surface. *Science*, **2011**, 334, 776-80	33.3	81
151	Imaging of the hydrogen subsurface site in rutile TiO2. *Physical Review Letters*, **2009**, 102, 136103	7.4	81
150	Formation and diffusion of water dimers on rutile TiO2(110). *Physical Review Letters*, **2009**, 102, 226101	7.4	80
149	Extended atomic hydrogen dimer configurations on the graphite(0001) surface. *Journal of Chemical Physics*, **2009**, 131, 084706	3.9	77
148	Dissociation path for H2 on Al(110). *Physical Review Letters*, **1992**, 69, 1971-1974	7.4	76
147	Covalent Interlinking of an Aldehyde and an Amine on a Au(111) Surface in Ultrahigh Vacuum. *Angewandte Chemie*, **2007**, 119, 9387-9390	3.6	75
146	Oxidation state of oxide supported nanometric gold. *Topics in Catalysis*, **2007**, 44, 49-56	2.3	73
145	Oxygen adsorption at anionic free and supported Au clusters. *Journal of Chemical Physics*, **2005**, 123, 161104	3.9	73
144	On-the-Fly Machine Learning of Atomic Potential in Density Functional Theory Structure Optimization. *Physical Review Letters*, **2018**, 120, 026102	7.4	72
143	CO Intercalation of Graphene on Ir(111) in the Millibar Regime. *Journal of Physical Chemistry C*, **2013**, 117, 16438-16447	3.8	70
142	Structure and activity of oxidized Pt(110) and alpha-PtO2. *Physical Chemistry Chemical Physics*, **2006**, 8, 1566-74	3.6	69
141	Adsorbate-induced alloy phase separation: a direct view by high-pressure scanning tunneling microscopy. *Physical Review Letters*, **2005**, 95, 126101	7.4	68
140	Nitrogen Adsorption and Hydrogenation on a MoFe6S9 Complex. *Physical Review Letters*, **1999**, 82, 4054-4057	7.4	68
139	Structure and catalytic reactivity of Rh oxides. *Catalysis Today*, **2009**, 145, 227-235	5.3	67
138	Steps on rutile TiO2(110): Active sites for water and methanol dissociation. *Physical Review B*, **2011**, 84,	3.3	66

137	Designing surface alloys with specific active sites. *Catalysis Letters*, **1996**, 40, 131-135	2.8	65
136	Inverted vibrational distributions from N2 recombination at Ru(001): Evidence for a metastable molecular chemisorption well. *Journal of Chemical Physics*, **1999**, 110, 6954-6962	3.9	64
135	A first-principles potential energy surface for Eley-Rideal reaction dynamics of H atoms on Cu(111). *Journal of Chemical Physics*, **1999**, 110, 2240-2249	3.9	64
134	Guanine Quartet Networks Stabilized by Cooperative Hydrogen Bonds. *Angewandte Chemie*, **2005**, 117, 2310-2315	3.6	63
133	The coupling between adsorption dynamics and the surface structure: H2 on Si(100). *Chemical Physics Letters*, **1994**, 229, 645-649	2.5	63
132	Controlling hydrogenation of graphene on Ir(111). *ACS Nano*, **2013**, 7, 3823-32	16.7	62
131	Coverage dependence of N2 dissociation at an N, O, or H precovered Ru(0001) surface investigated with density functional theory. *Physical Review B*, **2001**, 63,	3.3	62
130	Identification of the Catalytic Site at the Interface Perimeter of Au Clusters on Rutile TiO2(110). *ACS Catalysis*, **2014**, 4, 1626-1631	13.1	61
129	Density functional theory study of enantiospecific adsorption at chiral surfaces. *Journal of the American Chemical Society*, **2002**, 124, 14789-94	16.4	61
128	Comment on "High pressure adsorbate structures studied by scanning tunneling microscopy: CO on Pt(111) in equilibrium with the gas phase". *Physical Review Letters*, **2002**, 88, 259601	7.4	61
127	Adsorbate Reorganization at Steps: NO on Pd(211). *Physical Review Letters*, **1997**, 79, 4441-4444	7.4	60
126	Theory of Adsorption and Surface Reactions **1997**, 285-351		60
125	A surface coordination network based on copper adatom trimers. *Angewandte Chemie - International Edition*, **2014**, 53, 12955-9	16.4	58
124	Neural-network-enhanced evolutionary algorithm applied to supported metal nanoparticles. *Physical Review B*, **2018**, 97,	3.3	57
123	Graphene on metal surfaces and its hydrogen adsorption: A meta-GGA functional study. *Physical Review B*, **2012**, 86,	3.3	56
122	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	4.7	56
121	Role of steps in the dissociative adsorption of water on rutile TiO2(110). *Physical Review Letters*, **2013**, 110, 146101	7.4	54
120	Growth and electronic structure of epitaxial single-layer WS2 on Au(111). *Physical Review B*, **2015**, 92,	3.3	53

119	Direct evidence for ethanol dissociation on rutile TiO2(110). *Physical Review Letters*, **2011**, 107, 136102	7.4	53
118	Quantum-mechanical calculation of H on Ni(001) using a model potential based on first-principles calculations. *Physical Review B*, **1997**, 56, 2258-2266	3.3	53
117	Reactivity of a stepped surface NO dissociation on Pd(211). *Faraday Discussions*, **1998**, 110, 323-333	3.6	53
116	The interaction of hydrogen with the (110) surface of NiAl. *Surface Science*, **1995**, 331-333, 811-817	1.8	53
115	Promoting and poisoning effects of Na and Cl coadsorption on CO oxidation over MgO-supported Au nanoparticles. *Journal of Catalysis*, **2004**, 227, 217-226	7.3	52
114	Crystalline and electronic structure of single-layer TaS2. *Physical Review B*, **2016**, 94,	3.3	52
113	Treatment of Layered Structures Using a Semilocal meta-GGA Density Functional. *Journal of Physical Chemistry Letters*, **2010**, 1, 515-519	6.4	51
112	Probing enantioselectivity with x-ray photoelectron spectroscopy and density functional theory. *Physical Review Letters*, **2007**, 98, 136102	7.4	51
111	Visualizing hydrogen-induced reshaping and edge activation in MoS and Co-promoted MoS catalyst clusters. *Nature Communications*, **2018**, 9, 2211	17.4	50
110	An automated nudged elastic band method. *Journal of Chemical Physics*, **2016**, 145, 094107	3.9	50
109	Reactivity of a gas/metal/metal-oxide three-phase boundary: CO oxidation at the Pt(111)□(4□)-2CO/□PtO2 phase boundary. *Chemical Physics Letters*, **2005**, 409, 1-7	2.5	48
108	Stacking fault energies in aluminium. *Journal of Physics Condensed Matter*, **1992**, 4, 10453-10460	1.8	48
107	Guanine- and potassium-based two-dimensional coordination network self-assembled on Au(111). *Journal of the American Chemical Society*, **2010**, 132, 15927-9	16.4	46
106	Activation in prochiral reaction assemblies on Pt(111). *Journal of the American Chemical Society*, **2008**, 130, 5386-7	16.4	46
105	Atomic Energies from a Convolutional Neural Network. *Journal of Chemical Theory and Computation* , **2018**, 14, 3933-3942	6.4	45
104	□rratum to Electronic factors determining the reactivity of metal surfaces□[Surface Science 343 (1995) 211]. *Surface Science*, **1996**, 359, 306	1.8	43
103	The energetics and dynamics of H2 dissociation on Al(110). *Surface Science*, **1994**, 304, 131-144	1.8	43
102	Effect of subsurface Ti-interstitials on the bonding of small gold clusters on rutile TiO(2)(110). *Journal of Chemical Physics*, **2009**, 130, 044704	3.9	42

101	Structure and reactivity of a model catalyst alloy under realistic conditions. *Journal of Physics Condensed Matter*, **2008**, 20, 184018	1.8	42
100	CO Desorption Rate Dependence on CO Partial Pressure over Platinum Fuel Cell Catalysts. *Fuel Cells*, **2004**, 4, 309-319	2.9	42
99	Reduced step edges on rutile TiO2(110) as competing defects to oxygen vacancies on the terraces and reactive sites for ethanol dissociation. *Physical Review Letters*, **2012**, 109, 155501	7.4	41
98	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	3.8	41
97	Adsorbate-oxide interactions during the NO + CO reaction on MgO(100) supported Pd monolayer films. *Physical Review Letters*, **2002**, 89, 016102	7.4	41
96	Symmetry-Driven Band Gap Engineering in Hydrogen Functionalized Graphene. *ACS Nano*, **2016**, 10, 10798-10807	13.7	40
95	Theoretical study of H2O dissociation and CO oxidation on Pt2Mo(111). *Journal of Catalysis*, **2006**, 243, 192-198	7.3	40
94	Unravelling Site-Specific Photo-Reactions of Ethanol on Rutile TiO2(110). *Scientific Reports*, **2016**, 6, 21990	4.9	39
93	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	3.8	39
92	Structure and stability of small H clusters on graphene. *Physical Review B*, **2011**, 83,	3.3	39
91	Chemisorption and vibration of hydrogen on Cu(111). *Surface Science*, **1993**, 285, 27-30	1.8	39
90	Selective Propene Epoxidation on Immobilized Au6□10 Clusters: The Effect of Hydrogen and Water on Activity and Selectivity. *Angewandte Chemie*, **2009**, 121, 1495-1499	3.6	38
89	Efficient Global Structure Optimization with a Machine-Learned Surrogate Model. *Physical Review Letters*, **2020**, 124, 086102	7.4	37
88	Adsorption and dehydrogenation of tetrahydroxybenzene on Cu(111). *Chemical Communications*, **2013**, 49, 9308-10	5.8	37
87	Kinetics of fast island decay on Ag(111). *Physical Review B*, **2001**, 63,	3.3	37
86	An STM and DFT study of the ordered structures of NO on Pd(111). *Surface Science*, **2002**, 496, 1-9	1.8	37
85	Extended one-dimensional supramolecular assembly on a stepped surface. *Physical Review Letters*, **2008**, 100, 046103	7.4	36
84	A comparison of quantum and classical dynamics of H2 dissociation on Cu(111). *Surface Science*, **1996**, 364, 219-234	1.8	36

83	Combining Evolutionary Algorithms with Clustering toward Rational Global Structure Optimization at the Atomic Scale. *Journal of Chemical Theory and Computation*, **2017**, 13, 1486-1493	6.4	34
82	Stereodirection of an □ketoester at sub-molecular sites on chirally modified Pt(111): heterogeneous asymmetric catalysis. *Journal of the American Chemical Society*, **2013**, 135, 9999-10002	16.4	34
81	Self-consistent meta-generalized gradient approximation study of adsorption of aromatic molecules on noble metal surfaces. *Journal of Chemical Physics*, **2011**, 135, 084704	3.9	34
80	H2 dissociation at defected Cu: Preference for reaction at vacancy and kink sites. *Physical Review B*, **2002**, 65,	3.3	34
79	The mechanism of Mg conduction in ammine magnesium borohydride promoted by a neutral molecule. *Physical Chemistry Chemical Physics*, **2020**, 22, 9204-9209	3.6	33
78	Ethanol Diffusion on Rutile TiO2(110) Mediated by H Adatoms. *Journal of Physical Chemistry Letters* , **2012**, 3, 283-8	6.4	33
77	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	5.9	32
76	Dynamics of high-barrier surface reactions: laser-assisted associative desorption of N2 from Ru(0001). *Physical Review Letters*, **2000**, 84, 4906-9	7.4	31
75	Understanding intercalation structures formed under graphene on Ir(111). *Physical Review B*, **2014**, 90,	3.3	30
74	Comment on "Oxygen vacancy origin of the surface band-gap state of TiO2(110)". *Physical Review Letters*, **2010**, 104, 259703; author reply 259704	7.4	30
73	Exploration versus Exploitation in Global Atomistic Structure Optimization. *Journal of Physical Chemistry A*, **2018**, 122, 1504-1509	2.8	29
72	Adsorption properties versus oxidation states of rutile TiO2(110). *Journal of Chemical Physics*, **2011**, 134, 194703	3.9	29
71	Pyrene: hydrogenation, hydrogen evolution, and □band model. *Journal of Chemical Physics*, **2011**, 134, 164703	3.9	28
70	A Comparison of N2 and CO Adsorption on Ru(001). *Zeitschrift Fur Physikalische Chemie*, **1997**, 198, 113-122	3.1	27
69	Two-step reaction on a strained, nanoscale segmented surface. *Physical Review Letters*, **2004**, 93, 126104	7.4	27
68	Substrate-induced semiconductor-to-metal transition in monolayer WS2. *Physical Review B*, **2017**, 96,	3.3	26
67	Surface waves on NiAl(110). *Physical Review B*, **2001**, 63,	3.3	26
66	Remote Activation of Chemical Bonds in Heterogeneous Catalysis. *ACS Catalysis*, **2014**, 4, 1182-1188	13.1	25

65	Role of surface elastic relaxations in an O-induced nanopattern on Pt(110)-(1 x 2). *Physical Review Letters*, **2007**, 98, 115501	7.4	25
64	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	3.8	24
63	Water Dissociation and Hydroxyl Ordering on Anatase TiO_{2}(001)-(1□4). *Physical Review Letters*, **2018**, 121, 206003	7.4	24
62	Machine learning enhanced global optimization by clustering local environments to enable bundled atomic energies. *Journal of Chemical Physics*, **2018**, 149, 134104	3.9	24
61	Packing defects into ordered structures: strands on TiO2. *Physical Review Letters*, **2012**, 108, 236103	7.4	23
60	Band-gap engineering by Bi intercalation of graphene on Ir(111). *Physical Review B*, **2016**, 93,	3.3	22
59	Nucleation and growth of Pt nanoparticles on reduced and oxidized rutile TiO□(110). *Journal of Chemical Physics*, **2014**, 141, 214702	3.9	22
58	Theoretical investigation of the structure of □Al2O3. *Physical Review B*, **1997**, 55, 8721-8725	3.3	22
57	Atomistic structure learning. *Journal of Chemical Physics*, **2019**, 151, 054111	3.9	20
56	Structure determination of chemisorbed chirality transfer complexes: Accelerated STM analysis and exchange-correlation functional sensitivity. *Surface Science*, **2014**, 629, 48-56	1.8	20
55	CO oxidation on fully oxygen covered Ru(0001): Role of step edges. *Physical Review B*, **2010**, 81,	3.3	20
54	Enhanced Bonding of Silver Nanoparticles on Oxidized TiO2(110)□*Journal of Physical Chemistry C*, **2010**, 114, 16964-16972	3.8	20
53	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	3.9	20
52	Exciting H Molecules for Graphene Functionalization. *ACS Nano*, **2018**, 12, 513-520	16.7	19
51	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, 323-43	3.6	19
50	Tight-Binding Approximation-Enhanced Global Optimization. *Journal of Chemical Theory and Computation*, **2018**, 14, 2797-2807	6.4	18
49	Preservation of the Pt(100) surface reconstruction after growth of a continuous layer of graphene. *Surface Science*, **2012**, 606, 464-469	1.8	18
48	Adsorption, mobility, and dimerization of benzaldehyde on Pt(111). *Journal of Chemical Physics*, **2012**, 136, 174706	3.9	18

47	Walking-like diffusion of two-footed asymmetric aromatic adsorbates on Pt(111). *Surface Science*, **2014**, 629, 123-131	1.8	17
46	Tuning Aryl□H□□□O Intermolecular Interactions on Pt(111)□*Journal of Physical Chemistry C*, **2011**, 115, 1355-1360	3.8	17
45	Alkane dimers interaction: A semi-local MGGA functional study. *Chemical Physics Letters*, **2010**, 492, 183-186	2.3	17
44	Distinct reaction mechanisms in the catalytic oxidation of carbon monoxide on Rh(110): scanning tunneling microscopy and density functional theory studies. *Physical Review Letters*, **2001**, 87, 196104	7.4	17
43	Polarization and charge transfer during the dissociation of H2 on Al(110). *Surface Science*, **1993**, 297, L68-L72	1.8	17
42	Monitoring interconversion between stereochemical states in single chirality-transfer complexes on a platinum surface. *Nature Chemistry*, **2017**, 9, 531-536	17.6	16
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40	Accelerating atomic structure search with cluster regularization. *Journal of Chemical Physics*, **2018**, 148, 241734	3.9	15
39	Breakdown of the Graphene Coating Effect under Sequential Exposure to O2 and H2S. *Journal of Physical Chemistry Letters*, **2013**, 4, 3770-3774	6.4	14
38	Hydrogen bond rotations as a uniform structural tool for analyzing protein architecture. *Nature Communications*, **2014**, 5, 5803	17.4	14
37	Thermodynamic aspects of dehydrogenation reactions on noble metal surfaces. *Journal of Chemical Physics*, **2014**, 141, 174705	3.9	13
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