Bjrk Hammer

List of Publications by Year in Descending Order

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	Water Chemistry beneath Graphene: Condensation of a Dense OH-HO Phase under Graphene.. *Journal of Physical Chemistry C*, **2022**, 126, 4347-4354	3.8	0
225	Dimerization of dehydrogenated polycyclic aromatic hydrocarbons on graphene.. *Journal of Chemical Physics*, **2022**, 156, 134703	3.9	
224	Size-dependent phase stability in transition metal dichalcogenide nanoparticles controlled by metal substrates. *Nanoscale*, **2021**, 13, 10167-10180	7.7	2
223	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
222	Efficient Global Structure Optimization with a Machine-Learned Surrogate Model. *Physical Review Letters*, **2020**, 124, 086102	7.4	37
221	NH3 on anatase TiO2(101): Diffusion mechanisms and the effect of intermolecular repulsion. *Physical Review Materials*, **2020**, 4,	3.2	1
220	Structure prediction of surface reconstructions by deep reinforcement learning. *Journal of Physics Condensed Matter*, **2020**, 32, 404005	1.8	6
219	Gaussian representation for image recognition and reinforcement learning of atomistic structure. *Journal of Chemical Physics*, **2020**, 153, 044107	3.9	6
218	Atomistic structure learning algorithm with surrogate energy model relaxation. *Physical Review B*, **2020**, 102,	3.3	6
217	Chemically-resolved determination of hydrogenated graphene-substrate interaction. *Physical Chemistry Chemical Physics*, **2019**, 21, 13462-13466	3.6	5
216	Atomistic structure learning. *Journal of Chemical Physics*, **2019**, 151, 054111	3.9	20
215	Constructing convex energy landscapes for atomistic structure optimization. *Physical Review B*, **2019**, 100,	3.3	4
214	Effects of Gas-Phase Conditions and Particle Size on the Properties of Cu(111)-Supported ZnyOx Particles Revealed by Global Optimization and Ab Initio Thermodynamics. *Journal of Physical Chemistry C*, **2019**, 123, 30903-30916	3.8	5
213	Rotation and diffusion of naphthalene on Pt(111). *Journal of Chemical Physics*, **2018**, 148, 124703	3.9	2
212	Exciting H Molecules for Graphene Functionalization. *ACS Nano*, **2018**, 12, 513-520	16.7	19
211	On-the-Fly Machine Learning of Atomic Potential in Density Functional Theory Structure Optimization. *Physical Review Letters*, **2018**, 120, 026102	7.4	72
210	Exploration versus Exploitation in Global Atomistic Structure Optimization. *Journal of Physical Chemistry A*, **2018**, 122, 1504-1509	2.8	29

209	NH adsorption on anatase-TiO(101). *Journal of Chemical Physics*, **2018**, 148, 124704	3.9	7
208	Tight-Binding Approximation-Enhanced Global Optimization. *Journal of Chemical Theory and Computation*, **2018**, 14, 2797-2807	6.4	18
207	Visualizing hydrogen-induced reshaping and edge activation in MoS and Co-promoted MoS catalyst clusters. *Nature Communications*, **2018**, 9, 2211	17.4	50
206	Water Dissociation and Hydroxyl Ordering on Anatase TiO_{2}(001)-(1□). *Physical Review Letters*, **2018**, 121, 206003	7.4	24
205	An extended chiral surface coordination network based on Ag-clusters. *Journal of Chemical Physics*, **2018**, 149, 164710	3.9	10
204	Machine learning enhanced global optimization by clustering local environments to enable bundled atomic energies. *Journal of Chemical Physics*, **2018**, 149, 134104	3.9	24
203	Atomic Energies from a Convolutional Neural Network. *Journal of Chemical Theory and Computation* , **2018**, 14, 3933-3942	6.4	45
202	Neural-network-enhanced evolutionary algorithm applied to supported metal nanoparticles. *Physical Review B*, **2018**, 97,	3.3	57
201	Accelerating atomic structure search with cluster regularization. *Journal of Chemical Physics*, **2018**, 148, 241734	3.9	15
200	Water-Gas-Shift over Metal-Free Nanocrystalline Ceria: An Experimental and Theoretical Study. *ChemCatChem*, **2017**, 9, 1373-1377	5.2	12
199	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
198	Structure and Dynamics of Individual Diastereomeric Complexes on Platinum: Surface Studies Related to Heterogeneous Enantioselective Catalysis. *Accounts of Chemical Research*, **2017**, 50, 1163-1170	24.3	11
197	Monitoring interconversion between stereochemical states in single chirality-transfer complexes on a platinum surface. *Nature Chemistry*, **2017**, 9, 531-536	17.6	16
196	The atomic simulation environment-a Python library for working with atoms. *Journal of Physics Condensed Matter*, **2017**, 29, 273002	1.8	1097
195	Influence of CH□□N Interaction in the Self-Assembly of an Oligo(isoquinolyne-ethynylyne) Molecule with Distinct Conformational States. *Langmuir*, **2017**, 33, 10782-10791	4	2
194	Structure of the SnO_{2}(110)-(4□1) Surface. *Physical Review Letters*, **2017**, 119, 096102	7.4	16
193	Supramolecular Corrals on Surfaces Resulting from Aromatic Interactions of Nonplanar Triazoles. *ACS Nano*, **2017**, 11, 8302-8310	16.7	3
192	Substrate-induced semiconductor-to-metal transition in monolayer WS2. *Physical Review B*, **2017**, 96,	3.3	26

191	Band-gap engineering by Bi intercalation of graphene on Ir(111). *Physical Review B*, **2016**, 93,	3.3	22
190	Single-layer MoS2 on Au(111): Band gap renormalization and substrate interaction. *Physical Review B*, **2016**, 93,	3.3	93
189	Selection of conformational states in surface self-assembly for a molecule with eight possible pairs of surface enantiomers. *Chemical Communications*, **2016**, 52, 14023-14026	5.8	8
188	Symmetry-Driven Band Gap Engineering in Hydrogen Functionalized Graphene. *ACS Nano*, **2016**, 10, 10798-10807	13.7	40
187	Unravelling Site-Specific Photo-Reactions of Ethanol on Rutile TiO2(110). *Scientific Reports*, **2016**, 6, 21990	4.9	39
186	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
185	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	1.8	9
184	The influence of coronene super-hydrogenation on the coronene-graphite interaction. *Journal of Chemical Physics*, **2016**, 145, 174708	3.9	8
183	Pyridine adsorption and diffusion on Pt(111) investigated with density functional theory. *Journal of Chemical Physics*, **2016**, 144, 164112	3.9	12
182	Structure and role of metal clusters in a metal-organic coordination network determined by density functional theory. *Journal of Chemical Physics*, **2016**, 144, 084708	3.9	4
181	An automated nudged elastic band method. *Journal of Chemical Physics*, **2016**, 145, 094107	3.9	50
180	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
179	Crystalline and electronic structure of single-layer TaS2. *Physical Review B*, **2016**, 94,	3.3	52
178	In Situ Detection of Active Edge Sites in Single-Layer MoS2 Catalysts. *ACS Nano*, **2015**, 9, 9322-30	16.7	116
177	Isolating a Reaction Intermediate in the Hydrogenation of 2,2,2-Trifluoroacetophenone on Pt(111). *Journal of Physical Chemistry C*, **2015**, 119, 7319-7326	3.8	9
176	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	5.5	12
175	Selection of conformational states in self-assembled surface structures formed from an oligo(naphthylene-ethynylene) 3-bit binary switch. *Journal of Chemical Physics*, **2015**, 142, 101922	3.9	4
174	Growth and electronic structure of epitaxial single-layer WS2 on Au(111). *Physical Review B*, **2015**, 92,	3.3	53

173	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
172	Modeling Methyl Chloride Photo Oxidation by Oxygen Species on TiO2(110). *Topics in Catalysis*, **2014**, 57, 171-176	2.3	6
171	Remote Activation of Chemical Bonds in Heterogeneous Catalysis. *ACS Catalysis*, **2014**, 4, 1182-1188	13.1	25
170	A genetic algorithm for first principles global structure optimization of supported nano structures. *Journal of Chemical Physics*, **2014**, 141, 044711	3.9	122
169	A surface coordination network based on copper adatom trimers. *Angewandte Chemie - International Edition*, **2014**, 53, 12955-9	16.4	58
168	Structure determination of chemisorbed chirality transfer complexes: Accelerated STM analysis and exchange-correlation functional sensitivity. *Surface Science*, **2014**, 629, 48-56	1.8	20
167	Walking-like diffusion of two-footed asymmetric aromatic adsorbates on Pt(111). *Surface Science*, **2014**, 629, 123-131	1.8	17
166	Ein Metall-organisches Netzwerk auf Basis von Cu-Adatom- Trimeren. *Angewandte Chemie*, **2014**, 126, 13169-13173	3.6	11
165	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
164	Nucleation and growth of Pt nanoparticles on reduced and oxidized rutile TiO₂(110). *Journal of Chemical Physics*, **2014**, 141, 214702	3.9	22
163	Hydrogen bond rotations as a uniform structural tool for analyzing protein architecture. *Nature Communications*, **2014**, 5, 5803	17.4	14
162	Understanding intercalation structures formed under graphene on Ir(111). *Physical Review B*, **2014**, 90,	3.3	30
161	Thermodynamic aspects of dehydrogenation reactions on noble metal surfaces. *Journal of Chemical Physics*, **2014**, 141, 174705	3.9	13
160	Role of steps in the dissociative adsorption of water on rutile TiO2(110). *Physical Review Letters*, **2013**, 110, 146101	7.4	54
159	CO Intercalation of Graphene on Ir(111) in the Millibar Regime. *Journal of Physical Chemistry C*, **2013**, 117, 16438-16447	3.8	70
158	A density functional theory study of atomic steps on stoichiometric rutile TiO2(110). *Journal of Chemical Physics*, **2013**, 139, 234704	3.9	10
157	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
156	Adsorption and dehydrogenation of tetrahydroxybenzene on Cu(111). *Chemical Communications*, **2013**, 49, 9308-10	5.8	37

155	Controlling hydrogenation of graphene on Ir(111). *ACS Nano*, **2013**, 7, 3823-32	16.7	62
154	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
153	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
152	Interfacial oxygen under TiO2 supported Au clusters revealed by a genetic algorithm search. *Journal of Chemical Physics*, **2013**, 139, 204701	3.9	13
151	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
150	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
149	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, 92-6	6.4	10
148	Ethanol Diffusion on Rutile TiO2(110) Mediated by H Adatoms. *Journal of Physical Chemistry Letters* , **2012**, 3, 283-8	6.4	33
147	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
146	Preservation of the Pt(100) surface reconstruction after growth of a continuous layer of graphene. *Surface Science*, **2012**, 606, 464-469	1.8	18
145	Graphene on metal surfaces and its hydrogen adsorption: A meta-GGA functional study. *Physical Review B*, **2012**, 86,	3.3	56
144	Graphene coatings: probing the limits of the one atom thick protection layer. *ACS Nano*, **2012**, 6, 10258-66	16.7	81
143	Packing defects into ordered structures: strands on TiO2. *Physical Review Letters*, **2012**, 108, 236103	7.4	23
142	Linear hydrogen adsorbate structures on graphite induced by self-assembled molecular monolayers. *Carbon*, **2012**, 50, 2052-2056	10.4	12
141	Adsorption, mobility, and dimerization of benzaldehyde on Pt(111). *Journal of Chemical Physics*, **2012**, 136, 174706	3.9	18
140	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
139	Pyrene: hydrogenation, hydrogen evolution, and □band model. *Journal of Chemical Physics*, **2011**, 134, 164703	3.9	28
138	Steps on rutile TiO2(110): Active sites for water and methanol dissociation. *Physical Review B*, **2011**, 84,	3.3	66

137	Direct observation of molecular preorganization for chirality transfer on a catalyst surface. *Science*, **2011**, 334, 776-80	33.3	81
136	Structure and stability of small H clusters on graphene. *Physical Review B*, **2011**, 83,	3.3	39
135	Tuning Aryl□CH□□□O Intermolecular Interactions on Pt(111)□*Journal of Physical Chemistry C*, **2011**, 115, 1355-1360	3.8	17
134	Adsorption properties versus oxidation states of rutile TiO2(110). *Journal of Chemical Physics*, **2011**, 134, 194703	3.9	29
133	Direct evidence for ethanol dissociation on rutile TiO2(110). *Physical Review Letters*, **2011**, 107, 136102	7.4	53
132	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
131	Bandgap opening in graphene induced by patterned hydrogen adsorption. *Nature Materials*, **2010**, 9, 315-9	27	1229
130	Enevoldsen et al. Reply:. *Physical Review Letters*, **2010**, 104,	7.4	11
129	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
128	CO oxidation on fully oxygen covered Ru(0001): Role of step edges. *Physical Review B*, **2010**, 81,	3.3	20
127	DFT+U study of defects in bulk rutile TiO(2). *Journal of Chemical Physics*, **2010**, 133, 144708	3.9	114
126	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
125	Enhanced Bonding of Silver Nanoparticles on Oxidized TiO2(110)□*Journal of Physical Chemistry C*, **2010**, 114, 16964-16972	3.8	20
124	Treatment of Layered Structures Using a Semilocal meta-GGA Density Functional. *Journal of Physical Chemistry Letters*, **2010**, 1, 515-519	6.4	51
123	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
122	Water Adsorption on TiO2. *Topics in Catalysis*, **2010**, 53, 423-430	2.3	91
121	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
120	Alkane dimers interaction: A semi-local MGGA functional study. *Chemical Physics Letters*, **2010**, 492, 183-186	2.3	17

119	Imaging of the hydrogen subsurface site in rutile TiO2. *Physical Review Letters*, **2009**, 102, 136103	7.4	81
118	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
117	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
116	Structure and catalytic reactivity of Rh oxides. *Catalysis Today*, **2009**, 145, 227-235	5.3	67
115	Formation and diffusion of water dimers on rutile TiO2(110). *Physical Review Letters*, **2009**, 102, 226101	7.4	80
114	Extended atomic hydrogen dimer configurations on the graphite(0001) surface. *Journal of Chemical Physics*, **2009**, 131, 084706	3.9	77
113	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
112	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
111	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
110	The role of interstitial sites in the Ti3d defect state in the band gap of titania. *Science*, **2008**, 320, 1755-9	33.3	744
109	Activation in prochiral reaction assemblies on Pt(111). *Journal of the American Chemical Society*, **2008**, 130, 5386-7	16.4	46
108	Structure and reactivity of a model catalyst alloy under realistic conditions. *Journal of Physics Condensed Matter*, **2008**, 20, 184018	1.8	42
107	Extended one-dimensional supramolecular assembly on a stepped surface. *Physical Review Letters*, **2008**, 100, 046103	7.4	36
106	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
105	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
104	Oxidation state of oxide supported nanometric gold. *Topics in Catalysis*, **2007**, 44, 49-56	2.3	73
103	Probing enantioselectivity with x-ray photoelectron spectroscopy and density functional theory. *Physical Review Letters*, **2007**, 98, 136102	7.4	51
102	Enhanced bonding of gold nanoparticles on oxidized TiO2(110). *Science*, **2007**, 315, 1692-6	33.3	432

101	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
100	Theoretical study of H2O dissociation and CO oxidation on Pt2Mo(111). *Journal of Catalysis*, **2006**, 243, 192-198	7.3	40
99	Formation and splitting of paired hydroxyl groups on reduced TiO2(110). *Physical Review Letters*, **2006**, 96, 066107	7.4	362
98	Chiral recognition of organic molecules by atomic kinks on surfaces. *Physical Review Letters*, **2006**, 96, 056103	7.4	109
97	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
96	Metastable structures and recombination pathways for atomic hydrogen on the graphite (0001) surface. *Physical Review Letters*, **2006**, 96, 156104	7.4	278
95	Clustering of chemisorbed H(D) atoms on the graphite (0001) surface due to preferential sticking. *Physical Review Letters*, **2006**, 97, 186102	7.4	235
94	Structure and activity of oxidized Pt(110) and alpha-PtO2. *Physical Chemistry Chemical Physics*, **2006**, 8, 1566-74	3.6	69
93	Role of Au(+) in supporting and activating Au(7) on TiO(2)(110). *Physical Review Letters*, **2006**, 97, 136107	7.4	142
92	Chiral switching by spontaneous conformational change in adsorbed organic molecules. *Nature Materials*, **2006**, 5, 112-7	27	196
91	Special Sites at Noble and Late Transition Metal Catalysts. *Topics in Catalysis*, **2006**, 37, 3-16	2.3	235
90	The Role of the Chiral Modifier on the Enantioselective Hydrogenation of Methyl Pyruvate on Pt(111). *Catalysis Letters*, **2006**, 106, 111-114	2.8	12
89	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
88	One-dimensional PtO2 at Pt steps: formation and reaction with CO. *Physical Review Letters*, **2005**, 95, 256102	7.4	122
87	The activity of the tetrahedral Au20 cluster: charging and impurity effects. *Journal of Catalysis*, **2005**, 233, 399-404	7.3	122
86	Guanine quartet networks stabilized by cooperative hydrogen bonds. *Angewandte Chemie - International Edition*, **2005**, 44, 2270-5	16.4	262
85	Guanine Quartet Networks Stabilized by Cooperative Hydrogen Bonds. *Angewandte Chemie*, **2005**, 117, 2310-2315	3.6	63
84	Some recent theoretical advances in the understanding of the catalytic activity of Au. *Applied Catalysis A: General*, **2005**, 291, 21-31	5.1	222

83	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
82	The electronic structure effect in heterogeneous catalysis. *Catalysis Letters*, **2005**, 100, 111-114	2.8	253
81	Adsorbate-induced alloy phase separation: a direct view by high-pressure scanning tunneling microscopy. *Physical Review Letters*, **2005**, 95, 126101	7.4	68
80	Structure and reactivity of surface oxides on Pt(110) during catalytic CO oxidation. *Physical Review Letters*, **2005**, 95, 255505	7.4	305
79	Oxygen adsorption at anionic free and supported Au clusters. *Journal of Chemical Physics*, **2005**, 123, 161104	3.9	73
78	Two-step reaction on a strained, nanoscale segmented surface. *Physical Review Letters*, **2004**, 93, 126104	7.4	27
77	Oxidation of Pt(110). *Physical Review Letters*, **2004**, 93, 146104	7.4	122
76	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
75	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
74	CO Desorption Rate Dependence on CO Partial Pressure over Platinum Fuel Cell Catalysts. *Fuel Cells*, **2004**, 4, 309-319	2.9	42
73	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
72	Theoretical study of CO oxidation on Au nanoparticles supported by MgO(100). *Physical Review B*, **2004**, 69,	3.3	230
71	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
70	Active role of oxide support during CO oxidation at Au/MgO. *Physical Review Letters*, **2003**, 90, 206102	7.4	393
69	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
68	Chiral recognition in dimerization of adsorbed cysteine observed by scanning tunnelling microscopy. *Nature*, **2002**, 415, 891-3	50.4	529
67	Theoretical study of thiol-induced reconstructions on the Au(111) surface. *Chemical Physics Letters*, **2002**, 360, 264-271	2.5	155
66	Universality in Heterogeneous Catalysis. *Journal of Catalysis*, **2002**, 209, 275-278	7.3	1007

65	Density functional theory study of enantiospecific adsorption at chiral surfaces. *Journal of the American Chemical Society*, **2002**, 124, 14789-94	16.4	61
64	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
63	H2 dissociation at defected Cu: Preference for reaction at vacancy and kink sites. *Physical Review B*, **2002**, 65,	3.3	34
62	Adsorbate-oxide interactions during the NO + CO reaction on MgO(100) supported Pd monolayer films. *Physical Review Letters*, **2002**, 89, 016102	7.4	41
61	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
60	An STM and DFT study of the ordered structures of NO on Pd(111). *Surface Science*, **2002**, 496, 1-9	1.8	37
59	The Brønsted–Evans–Polanyi Relation and the Volcano Plot for Ammonia Synthesis over Transition Metal Catalysts. *Journal of Catalysis*, **2001**, 197, 229-231	7.3	471
58	The NO+CO Reaction Catalyzed by Flat, Stepped, and Edged Pd Surfaces. *Journal of Catalysis*, **2001**, 199, 171-176	7.3	125
57	Surface waves on NiAl(110). *Physical Review B*, **2001**, 63,	3.3	26
56	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
55	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
54	Kinetics of fast island decay on Ag(111). *Physical Review B*, **2001**, 63,	3.3	37
53	Oxygen dissociation at Pt steps. *Physical Review Letters*, **2001**, 87, 056103	7.4	178
52	The CO/Pt(111) Puzzle. *Journal of Physical Chemistry B*, **2001**, 105, 4018-4025	3.4	579
51	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
50	Adsorption, diffusion, and dissociation of NO, N and O on flat and stepped Ru(0001). *Surface Science*, **2000**, 459, 323-348	1.8	129
49	Theoretical surface science and catalysis—calculations and concepts. *Advances in Catalysis*, **2000**, 45, 71-129	2.4	1332
48	Bond Activation at Monatomic Steps: NO Dissociation at Corrugated Ru(0001). *Physical Review Letters*, **1999**, 83, 3681-3684	7.4	168

47	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
46	Nitrogen Adsorption and Hydrogenation on a MoFe6S9 Complex. *Physical Review Letters*, **1999**, 82, 4054-4057	7.4	68
45	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
44	Nitrogen Adsorption and Dissociation on Fe(111). *Journal of Catalysis*, **1999**, 182, 479-488	7.3	133
43	Improved adsorption energetics within density-functional theory using revised Perdew-Burke-Ernzerhof functionals. *Physical Review B*, **1999**, 59, 7413-7421	3.3	5077
42	Nitrogen adsorption on Fe(111), (100), and (110) surfaces. *Surface Science*, **1999**, 422, 8-16	1.8	88
41	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
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