

# Henrik Grønbeck

## List of Publications by Year in descending order

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216  
papers

10,808  
citations

36203

51  
h-index

37111

96  
g-index

222  
all docs

222  
docs citations

222  
times ranked

9666  
citing authors

#	ARTICLE	IF	CITATIONS
1	A unified view of ligand-protected gold clusters as superatom complexes. Proceedings of the National Academy of Sciences of the United States of America, 2008, 105, 9157-9162.	3.3	1,472
2	On the Structure of Thiolate-Protected Au <sub>25</sub> . Journal of the American Chemical Society, 2008, 130, 3756-3757.	6.6	682
3	Thiols and Disulfides on the Au(111) Surface: The Headgroup-Gold Interaction. Journal of the American Chemical Society, 2000, 122, 3839-3842.	6.6	591
4	Divide and Protect: Capping Gold Nanoclusters with Molecular Gold-Thiolate Rings. Journal of Physical Chemistry B, 2006, 110, 9927-9931.	1.2	405
5	Structure and Bonding in the Ubiquitous Icosahedral Metallic Gold Cluster Au <sub>144</sub> (SR) <sub>60</sub> . Journal of Physical Chemistry C, 2009, 113, 5035-5038.	1.5	393
6	The Active Phase of Palladium during Methane Oxidation. Journal of Physical Chemistry Letters, 2012, 3, 678-682.	2.1	183
7	Gold and platinum microclusters and their anions: comparison of structural and electronic properties. Chemical Physics, 2000, 262, 1-14.	0.9	149
8	CO Oxidation on Technological Pd <sub>2</sub> O <sub>3</sub> Catalysts: Oxidation State and Activity. Journal of Physical Chemistry C, 2011, 115, 1103-1111.	1.5	129
9	Gold-Thiolate Complexes Form a Unique $(4 \text{ \AA} - 2)$ Structure on Au(111). Journal of Physical Chemistry C, 2008, 112, 15940-15942.	1.5	125
10	Analysis of Porphyrines as Catalysts for Electrochemical Reduction of O <sub>2</sub> and Oxidation of H <sub>2</sub> O. Journal of the American Chemical Society, 2014, 136, 1320-1326.	6.6	124
11	Low Temperature CO Oxidation over Supported Ultrathin MgO Films. Journal of the American Chemical Society, 2009, 131, 16636-16637.	6.6	121
12	Theoretical Characterization of Cyclic Thiolated Gold Clusters. Journal of the American Chemical Society, 2006, 128, 10268-10275.	6.6	118
13	A Complete Multisite Reaction Mechanism for Low-Temperature NH <sub>3</sub> -SCR over Cu-CHA. ACS Catalysis, 2020, 10, 5646-5656.	5.5	118
14	Density functional theory approach to thiols and disulfides on gold: Au(111) surface and clusters. International Journal of Quantum Chemistry, 2000, 80, 598-608.	1.0	116
15	Thiolate-Protected Au <sub>25</sub> Superatoms as Building Blocks: Dimers and Crystals. Journal of Physical Chemistry C, 2010, 114, 15986-15994.	1.5	109
16	Methane Oxidation over PdO(101) Revealed by First-Principles Kinetic Modeling. Journal of the American Chemical Society, 2015, 137, 12035-12044.	6.6	104
17	Influence of atomic site-specific strain on catalytic activity of supported nanoparticles. Nature Communications, 2018, 9, 2722.	5.8	102
18	Chemistry of Supported Palladium Nanoparticles during Methane Oxidation. ACS Catalysis, 2015, 5, 2481-2489.	5.5	98

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19	NOx storage on BaO: theory and experiment. <i>Catalysis Today</i> , 2004, 96, 71-78.	2.2	91
20	Mechanism for NO <sub>2</sub> Charging on Metal Supported MgO. <i>Journal of Physical Chemistry B</i> , 2006, 110, 11977-11981.	1.2	91
21	Activation of oxygen on (NH <sub>3</sub> Cu NH <sub>3</sub> ) <sup>+</sup> in NH <sub>3</sub> -SCR over Cu-CHA. <i>Journal of Catalysis</i> , 2018, 358, 179-186.	3.1	91
22	Surface properties of alkaline earth metal oxides. <i>Surface Science</i> , 2004, 554, 262-271.	0.8	90
23	First-Principles Microkinetic Modeling of Methane Oxidation over Pd(100) and Pd(111). <i>ACS Catalysis</i> , 2016, 6, 6730-6738.	5.5	88
24	Methane oxidation over Pd and Pt studied by DFT and kinetic modeling. <i>Surface Science</i> , 2013, 616, 206-213.	0.8	87
25	Harmonic heat flow in isotropic layered systems and its use for thin film thermal conductivity measurements. <i>Journal of Applied Physics</i> , 1994, 75, 1914-1922.	1.1	85
26	Local Catalytic Ignition during CO Oxidation on Low-Index Pt and Pd Surfaces: A Combined PEEM, MS, and DFT Study. <i>Angewandte Chemie - International Edition</i> , 2012, 51, 10041-10044.	7.2	85
27	Oxidation and reduction of Pd(100) and aerosol-deposited Pd nanoparticles. <i>Physical Review B</i> , 2011, 83, .	1.1	79
28	Intrinsic Ligand Effect Governing the Catalytic Activity of Pd Oxide Thin Films. <i>ACS Catalysis</i> , 2014, 4, 3330-3334.	5.5	79
29	Charging of atoms, clusters, and molecules on metal-supported oxides: A general and long-ranged phenomenon. <i>Physical Review B</i> , 2008, 78, .	1.1	74
30	Mechanism for Limiting Thickness of Thin Oxide Films on Aluminum. <i>Physical Review Letters</i> , 2014, 112, 146103.	2.9	74
31	Scaling Relations and Kinetic Monte Carlo Simulations To Bridge the Materials Gap in Heterogeneous Catalysis. <i>ACS Catalysis</i> , 2017, 7, 5054-5061.	5.5	74
32	Characterization of NO <sub>x</sub> Species Adsorbed on BaO: Experiment and Theory. <i>Journal of Physical Chemistry B</i> , 2004, 108, 3523-3530.	1.2	73
33	Polymerization at the Alkylthiolate-Au(111) Interface. <i>Journal of Physical Chemistry B</i> , 2007, 111, 3325-3327.	1.2	73
34	Noble gas temperature control of metal clusters: A molecular dynamics study. <i>Journal of Chemical Physics</i> , 1997, 107, 3071-3079.	1.2	71
35	Adsorbate Entropies with Complete Potential Energy Sampling in Microkinetic Modeling. <i>Journal of Physical Chemistry C</i> , 2017, 121, 7199-7207.	1.5	70
36	Steps Control the Dissociation of CO <sub>2</sub> on Cu(100). <i>Journal of the American Chemical Society</i> , 2018, 140, 12974-12979.	6.6	70

#	ARTICLE	IF	CITATIONS
37	CO Adsorption on Clean and Oxidized Pd(111). <i>Journal of Physical Chemistry C</i> , 2014, 118, 1118-1128.	1.5	69
38	Geometric and electronic properties of small vanadium clusters: A density functional study. <i>Journal of Chemical Physics</i> , 1997, 107, 10620-10625.	1.2	67
39	Methane oxidation over alumina supported platinum investigated by time-resolved in situ XANES spectroscopy. <i>Journal of Catalysis</i> , 2007, 252, 11-17.	3.1	65
40	Selective Acetylene Hydrogenation over Single-Atom Alloy Nanoparticles by Kinetic Monte Carlo. <i>Journal of the American Chemical Society</i> , 2019, 141, 8541-8549.	6.6	63
41	Synthesis, characterization, electronic structure and catalytic performance of bimetallic and trimetallic nanoparticles containing tin. <i>Faraday Discussions</i> , 2008, 138, 301-315.	1.6	62
42	Promoting and poisoning effects of Na and Cl coadsorption on CO oxidation over MgO-supported Au nanoparticles. <i>Journal of Catalysis</i> , 2004, 227, 217-226.	3.1	61
43	Comparison of the bonding in Au <sub>8</sub> and Cu <sub>8</sub> : A density functional theory study. <i>Physical Review B</i> , 2005, 71, .	1.1	61
44	Real-time imaging of Na <sup>+</sup> reversible intercalation in Janus-graphene stacks for battery applications. <i>Science Advances</i> , 2021, 7, .	4.7	61
45	Vibrational study of ammonia adsorption on Pt/SiO <sub>2</sub> . <i>Applied Surface Science</i> , 2004, 235, 487-500.	3.1	60
46	Interpretation of NH <sub>3</sub> -TPD Profiles from Cu-CHA Using First-Principles Calculations. <i>Topics in Catalysis</i> , 2019, 62, 93-99.	1.3	60
47	Metal dimer sites in ZSM-5 zeolite for methane-to-methanol conversion from first-principles kinetic modelling: is the [Cu-O-Cu] <sup>2+</sup> motif relevant for Ni, Co, Fe, Ag, and Au?. <i>Catalysis Science and Technology</i> , 2017, 7, 1470-1477.	2.1	56
48	Oxidation of Small Silver Clusters: A Density Functional Theory Study. <i>Journal of Physical Chemistry C</i> , 2010, 114, 12610-12617.	1.5	55
49	Identifying surface species by vibrational spectroscopy: Bridging vs monodentate nitrates. <i>Journal of Catalysis</i> , 2008, 255, 127-133.	3.1	52
50	Catalytic hydrogenation of C=C and C=O in unsaturated fatty acid methyl esters. <i>Catalysis Science and Technology</i> , 2014, 4, 2427-2444.	2.1	52
51	Fundamental aspects of NO <sub>x</sub> adsorption on BaO. <i>Surface Science</i> , 2006, 600, 403-408.	0.8	51
52	Theoretical Characterization of Cyclic Thiolated Copper, Silver, and Gold Clusters. <i>Journal of Physical Chemistry C</i> , 2010, 114, 13571-13576.	1.5	51
53	On the Reaction Mechanism of Direct H <sub>2</sub> O <sub>2</sub> Formation over Pd Catalysts. <i>ACS Catalysis</i> , 2021, 11, 2735-2745.	5.5	50
54	Regenerable ceria-based SO <sub>x</sub> traps for sulfur removal in lean exhausts. <i>Applied Catalysis B: Environmental</i> , 2008, 84, 268-276.	10.8	49

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55	Size Effects in MgO Cube Dissolution. <i>Langmuir</i> , 2015, 31, 2770-2776.	1.6	49
56	The Site Assembly Determines Catalytic Activity of Nanoparticles. <i>Angewandte Chemie - International Edition</i> , 2018, 57, 5086-5089.	7.2	49
57	Methane oxidation over Pd/Al <sub>2</sub> O <sub>3</sub> under rich/lean cycling followed by operando XAFS and modulation excitation spectroscopy. <i>Journal of Catalysis</i> , 2017, 356, 237-245.	3.1	48
58	Effect of Al-distribution on oxygen activation over Cu-CHA. <i>Catalysis Science and Technology</i> , 2018, 8, 2131-2136.	2.1	47
59	High-Coverage Oxygen-Induced Surface Structures on Ag(111). <i>Journal of Physical Chemistry C</i> , 2014, 118, 15324-15331.	1.5	46
60	Investigation of niobium clusters: Bare and CO-adsorption. <i>Physical Review B</i> , 1996, 54, 1549-1552.	1.1	45
61	Structural, electronic, and vibrational properties of neutral and charged Nb <sub>n</sub> (n=8,9,10) clusters. <i>Physical Review A</i> , 1998, 58, 4630-4636.	1.0	44
62	Structural, Energetic, and Vibrational Properties of NO <sub>x</sub> Adsorption on Ag <sub>n</sub> , n= 1~8. <i>Journal of Physical Chemistry A</i> , 2007, 111, 6062-6067.	1.1	43
63	Study of Alkylthiolate Self-assembled Monolayers on Au(111) Using a Semilocal meta-GGA Density Functional. <i>Journal of Physical Chemistry C</i> , 2012, 116, 7374-7379.	1.5	43
64	Electro-oxidation of water on hematite: Effects of surface termination and oxygen vacancies investigated by first-principles. <i>Surface Science</i> , 2015, 640, 45-49.	0.8	43
65	Kinetic Regimes in Ethylene Hydrogenation over Transition-Metal Surfaces. <i>ACS Catalysis</i> , 2016, 6, 3277-3286.	5.5	43
66	Evidence of superatom electronic shells in ligand-stabilized aluminum clusters. <i>Journal of Chemical Physics</i> , 2011, 135, 094701.	1.2	42
67	Pt and Pt <sub>2</sub> on MgO(100) and BaO(100): structure, bonding, and chemical properties. <i>Journal of Chemical Physics</i> , 2003, 119, 3896-3904.	1.2	41
68	First Principles Studies of Metal-Oxide Surfaces. <i>Topics in Catalysis</i> , 2004, 28, 59-69.	1.3	41
69	The Al <sub>50</sub> Cp* <sub>12</sub> Cluster - A 138-Electron Closed Shell (L = 6) Superatom. <i>European Journal of Inorganic Chemistry</i> , 2011, 2011, 2649-2652.	1.0	41
70	A comparative test of different density functionals for calculations of NH <sub>3</sub> -SCR over Cu-Chabazite. <i>Physical Chemistry Chemical Physics</i> , 2019, 21, 10923-10930.	1.3	40
71	The Nature of NO <sub>x</sub> Species on BaO(100): An Ab Initio Molecular Dynamics Study. <i>Journal of Physical Chemistry B</i> , 2005, 109, 15410-15416.	1.2	39
72	Corrosion Induced Degradation of Pt/C Model Electrodes Measured with Electrochemical Quartz Crystal Microbalance. <i>Journal of the Electrochemical Society</i> , 2010, 157, B592.	1.3	39

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73	Structural and Energetic Trends of Ethylene Hydrogenation over Transition Metal Surfaces. Journal of Physical Chemistry C, 2016, 120, 995-1003.	1.5	39
74	High Specific and Mass Activity for the Oxygen Reduction Reaction for Thin Film Catalysts of Sputtered Pt <sub>3</sub> Y. Advanced Materials Interfaces, 2017, 4, 1700311.	1.9	39
75	CO on copper clusters: Orbital symmetry rules. Physical Review B, 1996, 53, 16644-16651.	1.1	38
76	Chemisorption on small clusters: can vertical detachment energy measurements provide chemical information? H on Au as a case study. Chemical Physics Letters, 2002, 361, 389-396.	1.2	38
77	Vibrational Analysis of H <sub>2</sub> and D <sub>2</sub> Adsorption on Pt/SiO <sub>2</sub> . Journal of Physical Chemistry B, 2005, 109, 9581-9588.	1.2	38
78	Thiolate Induced Reconstruction of Au(111) and Cu(111) Investigated by Density Functional Theory Calculations. Journal of Physical Chemistry C, 2010, 114, 15973-15978.	1.5	38
79	Understanding the Intrinsic Surface Reactivity of Single-Layer and Multilayer PdO(101) on Pd(100). ACS Catalysis, 2018, 8, 8553-8567.	5.5	38
80	Statistical theory of cluster cooling in rare gas. I. Energy transfer analysis for palladium clusters in helium. Journal of Chemical Physics, 1998, 109, 9848-9858.	1.2	37
81	Activity of Platinum/Carbon and Palladium/Carbon Catalysts Promoted by Ni <sub>2</sub> P in Direct Ethanol Fuel Cells. ChemSusChem, 2014, 7, 3374-3381.	3.6	37
82	CO-Induced Modification of the Metal/MgO(100) Interaction. Journal of Physical Chemistry B, 2003, 107, 12239-12243.	1.2	36
83	Transient Bimodal Particle Size Distributions during Pt Sintering on Alumina and Silica. Journal of Physical Chemistry C, 2015, 119, 989-996.	1.5	36
84	Strain Dependent Light-off Temperature in Catalysis Revealed by Planar Laser-Induced Fluorescence. ACS Catalysis, 2017, 7, 110-114.	5.5	36
85	First-Principles Studies of NO <sub>x</sub> Chemistry on Ag <sub>n</sub> /Al <sub>2</sub> O <sub>3</sub> . Journal of Physical Chemistry C, 2009, 113, 3674-3682.	1.5	35
86	Effect of lattice strain on hydrogen diffusion in Pd: A density functional theory study. Physical Review B, 2011, 84, .	1.1	35
87	Water Dissociation on MgO/Ag(100): Support Induced Stabilization or Electron Pairing?. Journal of Physical Chemistry C, 2010, 114, 7070-7075.	1.5	34
88	Mechanism for reversed photoemission core-level shifts of oxidized Ag. Physical Review B, 2012, 85, .	1.1	34
89	Surface composition of clean and oxidized Pd <sub>75</sub> Ag <sub>25</sub> (100) from photoelectron spectroscopy and density functional theory calculations. Surface Science, 2012, 606, 1777-1782.	0.8	34
90	Perspectives on Computational Catalysis for Metal Nanoparticles. ACS Catalysis, 2019, 9, 8872-8881.	5.5	34

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91	Mechanism for Solid-State Ion Exchange of Cu <sup>+</sup> into Zeolites. <i>Journal of Physical Chemistry C</i> , 2016, 120, 29182-29189.	1.5	33
92	Catalysis at the Rim: A Mechanism for Low Temperature CO Oxidation over Pt <sub>3</sub> Sn. <i>ACS Catalysis</i> , 2017, 7, 7431-7441.	5.5	32
93	Electrooxidation of Glycerol on Gold in Acidic Medium: A Combined Experimental and DFT Study. <i>Journal of Physical Chemistry C</i> , 2018, 122, 10489-10494.	1.5	32
94	Activation of $\text{Al}_2\text{O}_3$ by a Long-Ranged Chemical Bond Mechanism. <i>Physical Review Letters</i> , 2008, 100, 116801.	2.9	31
95	Reversed Hysteresis during CO Oxidation over Pd <sub>75</sub> Ag <sub>25</sub> (100). <i>ACS Catalysis</i> , 2016, 6, 4154-4161.	5.5	31
96	Visualizing catalyst heterogeneity by a multifrequential oscillating reaction. <i>Nature Communications</i> , 2018, 9, 600.	5.8	31
97	Tight-Binding Approximation-Enhanced Global Optimization. <i>Journal of Chemical Theory and Computation</i> , 2018, 14, 2797-2807.	2.3	31
98	Toward a Realistic Description of NO <sub>x</sub> Storage in BaO: The Aspect of BaCO <sub>3</sub> . <i>Journal of Physical Chemistry B</i> , 2005, 109, 9613-9621.	1.2	30
99	Effects of non-local exchange on core level shifts for gas-phase and adsorbed molecules. <i>Journal of Chemical Physics</i> , 2014, 141, 034706.	1.2	29
100	First Principles Calculations of Palladium Nanoparticle XANES Spectra. <i>Topics in Catalysis</i> , 2017, 60, 283-288.	1.3	28
101	The Role of H <sup>-</sup> and Cu <sup>+</sup> -Sites for N <sub>2</sub> O Formation during NH <sub>3</sub> -SCR over Cu-CHA. <i>Journal of Physical Chemistry C</i> , 2021, 125, 4595-4601.	1.5	28
102	Understanding the Phase Diagram of Self-Assembled Monolayers of Alkanethiolates on Gold. <i>Journal of Physical Chemistry C</i> , 2016, 120, 12059-12067.	1.5	27
103	Monte Carlo Potential Energy Sampling for Molecular Entropy in Zeolites. <i>Journal of Physical Chemistry C</i> , 2018, 122, 20351-20357.	1.5	27
104	Interplay between CO Disproportionation and Oxidation: On the Origin of the CO Reaction Onset on Atomic Layer Deposition-Grown Pt/ZrO <sub>2</sub> Model Catalysts. <i>ACS Catalysis</i> , 2021, 11, 208-214.	5.5	27
105	On the signatures of oxygen vacancies in O1s core level shifts. <i>Surface Science</i> , 2021, 705, 121761.	0.8	27
106	Phase Separation at the Nanoscale: Structural Properties of BaO Segregates on MgO-Based Nanoparticles. <i>Journal of Physical Chemistry C</i> , 2011, 115, 15853-15861.	1.5	26
107	Methane Oxidation Over Pd Supported on Ceria-Alumina Under Rich/Lean Cycling Conditions. <i>Topics in Catalysis</i> , 2013, 56, 410-415.	1.3	26
108	2D-3D structural transition in sub-nanometer Pt <sub>N</sub> clusters supported on CeO <sub>2</sub> (111). <i>Physical Chemistry Chemical Physics</i> , 2017, 19, 17845-17855.	1.3	26

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109	MonteCoffee: A programmable kinetic Monte Carlo framework. Journal of Chemical Physics, 2018, 149, 114101.	1.2	26
110	Dissociative Adsorption of Hydrogen on PdO(101) Studied by HRCLS and DFT. Journal of Physical Chemistry C, 2013, 117, 13510-13519.	1.5	25
111	First-Principles Microkinetic Model for Low-Temperature NH <sub>3</sub> -Assisted Selective Catalytic Reduction of NO over Cu-CHA. ACS Catalysis, 2021, 11, 14395-14407.	5.5	25
112	Tunable Ti <sup>3+</sup> -Mediated Charge Carrier Dynamics of Atomic Layer Deposition-Grown Amorphous TiO <sub>2</sub> . Journal of Physical Chemistry C, 2022, 126, 4542-4554.	1.5	25
113	A Chemical View on X-ray Photoelectron Spectroscopy: the ESCA Molecule and Surface to Bulk XPS Shifts. ChemPhysChem, 2018, 19, 169-174.	1.0	24
114	CO <sub>2</sub> adsorption on hydroxylated In <sub>2</sub> O <sub>3</sub> (110). Physical Chemistry Chemical Physics, 2019, 21, 21698-21708.	1.3	23
115	Experimental and theoretical characterization of NO <sub>x</sub> species on Ag/Al <sub>2</sub> O <sub>3</sub> . Journal of Molecular Catalysis A, 2009, 314, 102-109.	4.8	22
116	Thermal Stability of Single-Crystalline IrO <sub>2</sub> (110) Layers: Spectroscopic and Adsorption Studies. Journal of Physical Chemistry C, 2020, 124, 15324-15336.	1.5	22
117	Resolving multifrequential oscillations and nanoscale interfacet communication in single-particle catalysis. Science, 2021, 372, 1314-1318.	6.0	22
118	<i>Ab initio</i> molecular dynamics calculations of $H_2O$ on BaO(001). Physical Review B, 2008, 77, .	1.1	21
119	H <sub>2</sub> dissociation over Ag/Al <sub>2</sub> O <sub>3</sub> : the first step in hydrogen assisted selective catalytic reduction of NO <sub>x</sub> . Catalysis Science and Technology, 2013, 3, 183-190.	2.1	21
120	Trends in adsorbate induced core level shifts. Surface Science, 2015, 640, 59-64.	0.8	21
121	Adsorption of NO on Fe <sub>3</sub> O <sub>4</sub> (111). Chemical Physics Letters, 2018, 693, 84-87.	1.2	21
122	Hydrogen adsorption on In <sub>2</sub> O <sub>3</sub> (111) and In <sub>2</sub> O <sub>3</sub> (110). Physical Chemistry Chemical Physics, 2020, 22, 16193-16202.	1.3	21
123	Photoemission core-level shifts reveal the thiolate-Au(111) interface. Physical Review B, 2010, 82, .	1.1	20
124	Carbonate formation on $p_4\bar{1}$ Physical Review B, 2011, 84, .	1.1	20
125	Exceptionally Active Single-Site Nanocluster Multifunctional Catalysts for Cascade Reactions. ChemCatChem, 2010, 2, 402-406.	1.8	19
126	A First-Principles-Based Microkinetic Study of CO <sub>2</sub> Reduction to CH <sub>3</sub> OH over In <sub>2</sub> O <sub>3</sub> (110). ACS Catalysis, 2021, 11, 9996-10006.	5.5	19



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127	Analysis of the odd-even alternation in simple metal clusters. Zeitschrift für Physik D-Atoms Molecules and Clusters, 1996, 36, 153-157.	1.0	18
128	In Situ Plasmonic Sensing of Platinum Model Catalyst Sintering on Different Oxide Supports and in O <sub>2</sub> and NO <sub>2</sub> Atmospheres with Different Concentrations. ACS Catalysis, 2015, 5, 426-432.	5.5	18
129	Plasmonic Nanospectroscopy of Platinum Catalyst Nanoparticle Sintering in a Mesoporous Alumina Support. ACS Nano, 2016, 10, 5063-5069.	7.3	18
130	Thin water films and particle morphology evolution in nanocrystalline MgO. Journal of the American Ceramic Society, 2018, 101, 4994-5003.	1.9	18
131	Surface-Structure Libraries: Multifrequential Oscillations in Catalytic Hydrogen Oxidation on Rhodium. Journal of Physical Chemistry C, 2019, 123, 4217-4227.	1.5	18
132	Does hydrogen pre-melt palladium clusters?. Chemical Physics Letters, 1997, 264, 39-43.	1.2	17
133	Characterization of Iron Carbonyl-Protected Gold Clusters. Journal of the American Chemical Society, 2009, 131, 12573-12575.	6.6	17
134	Modelling complete methane oxidation over palladium oxide in a porous catalyst using first-principles surface kinetics. Catalysis Science and Technology, 2018, 8, 508-520.	2.1	17
135	Initial oxidation of Cu(100) studied by X-ray photo-electron spectroscopy and density functional theory calculations. Surface Science, 2018, 675, 64-69.	0.8	17
136	First-Principles Study of Oxidation State and Coordination of Cu-Dimers in Cu-SSZ-13 during Methane-to-Methanol Reaction Conditions. Journal of Physical Chemistry C, 2019, 123, 26145-26150.	1.5	17
137	Effects of the metal in the adsorption of NO <sub>2</sub> on platinum supported BaO films. Surface Science, 2006, 600, L214-L218.	0.8	16
138	NO <sub>2</sub> dissociation on Ag(111) revisited by theory. Journal of Chemical Physics, 2008, 128, 104704.	1.2	16
139	The bonding in thiolate protected gold nanoparticles from Au4f photoemission core level shifts. Nanoscale, 2012, 4, 4178.	2.8	16
140	Water desorption from nanostructured graphite surfaces. Physical Chemistry Chemical Physics, 2013, 15, 20456.	1.3	16
141	Tuning the Reactivity of Ultrathin Oxides: NO Adsorption on Monolayer FeO(111). Angewandte Chemie - International Edition, 2016, 55, 9267-9271.	7.2	16
142	Pt Nanoparticle Sintering and Redispersion on a Heterogeneous Nanostructured Support. Journal of Physical Chemistry C, 2016, 120, 14918-14925.	1.5	16
143	Unraveling the Surface Chemistry and Structure in Highly Active Sputtered Pt <sub>3</sub> Y Catalyst Films for the Oxygen Reduction Reaction. ACS Applied Materials & Interfaces, 2020, 12, 4454-4462.	4.0	16
144	A jellium approach to the chemisorption of molecular oxygen on copper clusters. Chemical Physics Letters, 1994, 227, 149-156.	1.2	15

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145	Simulated Photoemission Spectra of Hydroxylated MgO(100) at Elevated Temperatures. Journal of Physical Chemistry C, 2012, 116, 3545-3551.	1.5	15
146	Efficient hydrogenation over single-site bimetallic RuSn clusters. Physical Chemistry Chemical Physics, 2013, 15, 9694.	1.3	15
147	Cluster Size Effects in Ethylene Hydrogenation over Palladium. Journal of Physical Chemistry C, 2017, 121, 10870-10875.	1.5	15
148	Revealing Carbon Phenomena at Palladium Nanoparticles by Analyzing the Work Function. Journal of Physical Chemistry C, 2019, 123, 4360-4370.	1.5	15
149	Theoretical study of (CO) <sub>n</sub> chemisorption on Pt and Pt <sub>3</sub> : structural, electronic and vibrational properties. Chemical Physics Letters, 1997, 269, 385-390.	1.2	14
150	Oxidation at the Subnanometer Scale. Journal of Physical Chemistry C, 2015, 119, 10797-10803.	1.5	14
151	Selectivity and kinetics of methyl crotonate hydrogenation over Pt/Al <sub>2</sub> O <sub>3</sub> . Catalysis Science and Technology, 2015, 5, 1716-1730.	2.1	14
152	Connection between macroscopic kinetic measurables and the degree of rate control. Catalysis Science and Technology, 2017, 7, 4034-4040.	2.1	14
153	Fuel Cell Measurements with Cathode Catalysts of Sputtered Pt <sub>3</sub> Y Thin Films. ChemSusChem, 2018, 11, 1438-1445.	3.6	14
154	Oxygen step-response experiments for methane oxidation over Pd/Al <sub>2</sub> O <sub>3</sub> : An in situ XAFS study. Catalysis Communications, 2018, 109, 24-27.	1.6	14
155	Theoretical study of chemisorption on niobium clusters: carbon monoxide and oxygen. Zeitschrift für Physik D-Atoms Molecules and Clusters, 1997, 40, 206-209.	1.0	13
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