Henrik GrÃ¶nbeck

List of Publications by Year in descending order

216 papers	10,808 citations	36303 51 h-index	37204 96 g-index
222 all docs	222 docs citations	222 times ranked	9666 citing authors

#	Article	IF	Citations
1	Can oxygen vacancies in ceria surfaces be measured by O1s photoemission spectroscopy?. Journal of Physics Condensed Matter, 2022, 34, 174004.	1.8	11
2	Surface steps dominate the water formation on Pd(111) surfaces. Journal of Chemical Physics, 2022, 156, 064701.	3.0	8
3	Tunable Ti³⁺-Mediated Charge Carrier Dynamics of Atomic Layer Deposition-Grown Amorphous TiO₂. Journal of Physical Chemistry C, 2022, 126, 4542-4554.	3.1	25
4	Probing the role of grain boundaries in single Cu nanoparticle oxidation by in situ plasmonic scattering. Physical Review Materials, 2022, 6, .	2.4	4
5	In situ DRIFT studies on N₂O formation over Cu-functionalized zeolites during ammonia-SCR. Catalysis Science and Technology, 2022, 12, 3921-3936.	4.1	4
6	Interplay between CO Disproportionation and Oxidation: On the Origin of the CO Reaction Onset on Atomic Layer Deposition-Grown Pt/ZrO₂ Model Catalysts. ACS Catalysis, 2021, 11, 208-214.	11.2	27
7	On the signatures of oxygen vacancies in O1s core level shifts. Surface Science, 2021, 705, 121761.	1.9	27
8	Role of hydroxylation for the atomic structure of a non-polar vicinal zinc oxide. Communications Chemistry, 2021, 4, .	4.5	6
9	On the Reaction Mechanism of Direct H₂O₂ Formation over Pd Catalysts. ACS Catalysis, 2021, 11, 2735-2745.	11.2	50
10	The Role of H⁺- and Cu⁺-Sites for N₂O Formation during NH₃-SCR over Cu-CHA. Journal of Physical Chemistry C, 2021, 125, 4595-4601.	3.1	28
11	Real-time imaging of Na ⁺ reversible intercalation in â€œJanusâ€•graphene stacks for battery applications. Science Advances, 2021, 7, .	10.3	61
12	Resolving multifrequential oscillations and nanoscale interfacet communication in single-particle catalysis. Science, 2021, 372, 1314-1318.	12.6	22
13	Direct measurement of enthalpy and entropy changes in NH 3 promoted O 2 activation over Cuâ^'CHA at low temperature. ChemCatChem, 2021, 13, 2577-2582.	3.7	11
14	Complete Reaction Cycle for Methane-to-Methanol Conversion over Cu-SSZ-13: First-Principles Calculations and Microkinetic Modeling. Journal of Physical Chemistry C, 2021, 125, 14681-14688.	3.1	10
15	A First-Principles-Based Microkinetic Study of CO₂ Reduction to CH₃OH over In₂O₃(110). ACS Catalysis, 2021, 11, 9996-10006.	11.2	19
16	Single-Particle Catalysis: Revealing Intraparticle Pacemakers in Catalytic H₂ Oxidation on Rh. ACS Catalysis, 2021, 11, 10020-10027.	11.2	9
17	Reduced Carbon Monoxide Saturation Coverage on Vicinal Palladium Surfaces: the Importance of the Adsorption Site. Journal of Physical Chemistry Letters, 2021, 12, 9508-9515.	4.6	3
18	Reaction Mechanism for Methane-to-Methanol in Cu-SSZ-13: First-Principles Study of the Z2[Cu2O] and Z2[Cu2OH] Motifs. Catalysts, 2021, 11, 17.	3.5	2

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19	Coexisting multi-states in catalytic hydrogen oxidation on rhodium. Nature Communications, 2021, 12, 6517.	12.8	5
20	First-Principles Microkinetic Model for Low-Temperature NH₃-Assisted Selective Catalytic Reduction of NO over Cu-CHA. ACS Catalysis, 2021, 11, 14395-14407.	11.2	25
21	Unraveling the Surface Chemistry and Structure in Highly Active Sputtered Pt₃Y Catalyst Films for the Oxygen Reduction Reaction. ACS Applied Materials & Interfaces, 2020, 12, 4454-4462.	8.0	16
22	Structureâ€Ðependent Strain Effects. ChemPhysChem, 2020, 21, 2407-2410.	2.1	11
23	Thermal Stability of Single-Crystalline IrO₂(110) Layers: Spectroscopic and Adsorption Studies. Journal of Physical Chemistry C, 2020, 124, 15324-15336.	3.1	22
24	Sensitivity of Monte Carlo Simulations to Linear Scaling Relations. Journal of Physical Chemistry C, 2020, 124, 11952-11959.	3.1	5
25	Structure of two-dimensional Fe3O4. Journal of Chemical Physics, 2020, 152, 114705.	3.0	10
26	Hydrogen adsorption on In₂O₃(111) and In₂O₃(110). Physical Chemistry Chemical Physics, 2020, 22, 16193-16202.	2.8	21
27	A Complete Multisite Reaction Mechanism for Low-Temperature NH₃-SCR over Cu-CHA. ACS Catalysis, 2020, 10, 5646-5656.	11.2	118
28	Stability, magnetic order, and electronic properties of ultrathin <mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mrow><mml:msub><mml:mi>Fe</mml:mi><mml:mn>3</mml:mn></mml:r mathvariant="normal">O</mml:mi><mml:mn>4</mml:mn></mml:msub></mml:mrow></mml:math> nanosheets. Physical Review B, 2020, 101, .	3.2	3
29	Perspectives on Computational Catalysis for Metal Nanoparticles. ACS Catalysis, 2019, 9, 8872-8881.	11.2	34
30	CO2 adsorption on hydroxylated In2O3(110). Physical Chemistry Chemical Physics, 2019, 21, 21698-21708.	2.8	23
31	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.	3.1	17
32	Strain Affects CO Oxidation on Metallic Nanoparticles Non-linearly. Topics in Catalysis, 2019, 62, 660-668.	2.8	9
33	Oxygen Adsorption on Graphene-Encapsulated Palladium Nanoparticles Imaged by Kelvin Probe Force Microscopy. Journal of Physical Chemistry C, 2019, 123, 24615-24625.	3.1	6
34	A dimer path for CO dissociation on PtSn. Catalysis Science and Technology, 2019, 9, 695-701.	4.1	9
35	Revealing Carbon Phenomena at Palladium Nanoparticles by Analyzing the Work Function. Journal of Physical Chemistry C, 2019, 123, 4360-4370.	3.1	15
36	Initial Fe₃O₄(100) Formation on Fe(100). Journal of Physical Chemistry C, 2019, 123, 16317-16325.	3.1	8

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37	Selective Acetylene Hydrogenation over Single-Atom Alloy Nanoparticles by Kinetic Monte Carlo. Journal of the American Chemical Society, 2019, 141, 8541-8549.	13.7	63
38	A comparative test of different density functionals for calculations of NH₃-SCR over Cu-Chabazite. Physical Chemistry Chemical Physics, 2019, 21, 10923-10930.	2.8	40
39	Multiscale reactor modelling of total pressure effects on complete methane oxidation over Pd/Al₂O₃. Catalysis Science and Technology, 2019, 9, 3055-3065.	4.1	3
40	Surface-Structure Libraries: Multifrequential Oscillations in Catalytic Hydrogen Oxidation on Rhodium. Journal of Physical Chemistry C, 2019, 123, 4217-4227.	3.1	18
41	Correlation between Ethylene Adsorption Energies and Core-Level Shifts for Pd Nanoclusters. Journal of Physical Chemistry C, 2019, 123, 2544-2548.	3.1	3
42	Interpretation of NH3-TPD Profiles from Cu-CHA Using First-Principles Calculations. Topics in Catalysis, 2019, 62, 93-99.	2.8	60
43	Fuel Cell Measurements with Cathode Catalysts of Sputtered Pt₃Y Thin Films. ChemSusChem, 2018, 11, 1438-1445.	6.8	14
44	The Siteâ€Assembly Determines Catalytic Activity of Nanoparticles. Angewandte Chemie, 2018, 130, 5180-5183.	2.0	4
45	The Siteâ€Assembly Determines Catalytic Activity of Nanoparticles. Angewandte Chemie - International Edition, 2018, 57, 5086-5089.	13.8	49
46	Electrooxidation of Glycerol on Gold in Acidic Medium: A Combined Experimental and DFT Study. Journal of Physical Chemistry C, 2018, 122, 10489-10494.	3.1	32
47	Seâ€“C Cleavage of Hexane Selenol at Steps on Au(111). Langmuir, 2018, 34, 2630-2636.	3.5	2
48	Adsorption of NO on Fe3O4(111). Chemical Physics Letters, 2018, 693, 84-87.	2.6	21
49	Visualizing catalyst heterogeneity by a Âmultifrequential oscillating reaction. Nature Communications, 2018, 9, 600.	12.8	31
50	A Chemical View on Xâ€ray Photoelectron Spectroscopy: the ESCA Molecule and Surfaceâ€toâ€Bulk XPS Shifts. ChemPhysChem, 2018, 19, 169-174.	2.1	24
51	Activation of oxygen on (NH3Cu NH3)+ in NH3-SCR over Cu-CHA. Journal of Catalysis, 2018, 358, 179-186.	6.2	91
52	Fuel Cell Measurements with Cathode Catalysts of Sputtered Pt3 Y Thin Films. ChemSusChem, 2018, 11, 1394-1394.	6.8	0
53	Oxygen step-response experiments for methane oxidation over Pd/Al2O3: An in situ XAFS study. Catalysis Communications, 2018, 109, 24-27.	3.3	14
54	Tight-Binding Approximation-Enhanced Global Optimization. Journal of Chemical Theory and Computation, 2018, 14, 2797-2807.	5.3	31

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55	Effect of Al-distribution on oxygen activation over Cuâ€“CHA. Catalysis Science and Technology, 2018, 8, 2131-2136.	4.1	47
56	The Influence of Inert Ions on the Reactivity of Manganese Oxides. Journal of Physical Chemistry C, 2018, 122, 216-226.	3.1	11
57	Modelling complete methane oxidation over palladium oxide in a porous catalyst using first-principles surface kinetics. Catalysis Science and Technology, 2018, 8, 508-520.	4.1	17
58	Extracting Local Quantitative Atomic-resolution Strain Information from High-precision STEM Data of Supported Nanocatalysts. Microscopy and Microanalysis, 2018, 24, 52-53.	0.4	0
59	MonteCoffee: A programmable kinetic Monte Carlo framework. Journal of Chemical Physics, 2018, 149, 114101.	3.0	26
60	CO Oxidation at SnO2/Pt3Sn(111) Interfaces. Topics in Catalysis, 2018, 61, 1458-1464.	2.8	4
61	Steps Control the Dissociation of CO₂ on Cu(100). Journal of the American Chemical Society, 2018, 140, 12974-12979.	13.7	70
62	Initial oxidation of Cu(100) studied by X-ray photo-electron spectroscopy and density functional theory calculations. Surface Science, 2018, 675, 64-69.	1.9	17
63	Thin water films and particle morphology evolution in nanocrystalline MgO. Journal of the American Ceramic Society, 2018, 101, 4994-5003.	3.8	18
64	Understanding the Intrinsic Surface Reactivity of Single-Layer and Multilayer PdO(101) on Pd(100). ACS Catalysis, 2018, 8, 8553-8567.	11.2	38
65	Influence of atomic site-specific strain on catalytic activity of supported nanoparticles. Nature Communications, 2018, 9, 2722.	12.8	102
66	Monte Carlo Potential Energy Sampling for Molecular Entropy in Zeolites. Journal of Physical Chemistry C, 2018, 122, 20351-20357.	3.1	27
67	First Principles Calculations of Palladium Nanoparticle XANES Spectra. Topics in Catalysis, 2017, 60, 283-288.	2.8	28
68	Metal dimer sites in ZSM-5 zeolite for methane-to-methanol conversion from first-principles kinetic modelling: is the [Cuâ€“Oâ€“Cu]²⁺motif relevant for Ni, Co, Fe, Ag, and Au?. Catalysis Science and Technology, 2017, 7, 1470-1477.	4.1	56
69	Cluster Size Effects in Ethylene Hydrogenation over Palladium. Journal of Physical Chemistry C, 2017, 121, 10870-10875.	3.1	15
70	High Specific and Mass Activity for the Oxygen Reduction Reaction for Thin Film Catalysts of Sputtered Pt₃Y. Advanced Materials Interfaces, 2017, 4, 1700311.	3.7	39
71	Scaling Relations and Kinetic Monte Carlo Simulations To Bridge the Materials Gap in Heterogeneous Catalysis. ACS Catalysis, 2017, 7, 5054-5061.	11.2	74
72	2Dâ€“3D structural transition in sub-nanometer Pt_N clusters supported on CeO₂(111). Physical Chemistry Chemical Physics, 2017, 19, 17845-17855.	2.8	26

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73	Threeâ€Dimensional Probing of Catalyst Ageing on Different Length Scales: A Case Study of Changes in Microstructure and Activity for CO Oxidation of a Ptâ€“Pd/Al₂O₃ Catalyst. ChemCatChem, 2017, 9, 3544-3553.	3.7	2
74	Adsorbate Entropies with Complete Potential Energy Sampling in Microkinetic Modeling. Journal of Physical Chemistry C, 2017, 121, 7199-7207.	3.1	70
75	Adsorbate Pairing on Oxide Surfaces: Influence on Reactivity and Dependence on Oxide, Adsorbate Pair, and Density Functional. Journal of Physical Chemistry C, 2017, 121, 8390-8398.	3.1	12
76	Catalysis at the Rim: A Mechanism for Low Temperature CO Oxidation over Pt₃Sn. ACS Catalysis, 2017, 7, 7431-7441.	11.2	32
77	Fuel Cells: High Specific and Mass Activity for the Oxygen Reduction Reaction for Thin Film Catalysts of Sputtered Pt₃Y (Adv. Mater. Interfaces 13/2017). Advanced Materials Interfaces, 2017, 4, .	3.7	0
78	Connection between macroscopic kinetic measurables and the degree of rate control. Catalysis Science and Technology, 2017, 7, 4034-4040.	4.1	14
79	Methane oxidation over Pd/Al2O3 under rich/lean cycling followed by operando XAFS and modulation excitation spectroscopy. Journal of Catalysis, 2017, 356, 237-245.	6.2	48
80	Fe Oxides on Ag Surfaces: Structure and Reactivity. Topics in Catalysis, 2017, 60, 492-502.	2.8	10
81	Strain Dependent Light-off Temperature in Catalysis Revealed by Planar Laser-Induced Fluorescence. ACS Catalysis, 2017, 7, 110-114.	11.2	36
82	Correspondence: On the bonding in ligand-protected gold clusters. Nature Communications, 2017, 8, 1612.	12.8	4
83	Tuning the Reactivity of Ultrathin Oxides: NO Adsorption on Monolayer FeO(111). Angewandte Chemie, 2016, 128, 9413-9417.	2.0	2
84	Mechanism for Solid-State Ion Exchange of Cu⁺ into Zeolites. Journal of Physical Chemistry C, 2016, 120, 29182-29189.	3.1	33
85	Reversed Hysteresis during CO Oxidation over Pd75Ag25(100). ACS Catalysis, 2016, 6, 4154-4161.	11.2	31
86	Kinetic Regimes in Ethylene Hydrogenation over Transition-Metal Surfaces. ACS Catalysis, 2016, 6, 3277-3286.	11.2	43
87	Plasmonic Nanospectroscopy of Platinum Catalyst Nanoparticle Sintering in a Mesoporous Alumina Support. ACS Nano, 2016, 10, 5063-5069.	14.6	18
88	Tuning the Reactivity of Ultrathin Oxides: NO Adsorption on Monolayer FeO(111). Angewandte Chemie - International Edition, 2016, 55, 9267-9271.	13.8	16
89	First-Principles Microkinetic Modeling of Methane Oxidation over Pd(100) and Pd(111). ACS Catalysis, 2016, 6, 6730-6738.	11.2	88
90	Understanding the Phase Diagram of Self-Assembled Monolayers of Alkanethiolates on Gold. Journal of Physical Chemistry C, 2016, 120, 12059-12067.	3.1	27

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91	Pt Nanoparticle Sintering and Redispersion on a Heterogeneous Nanostructured Support. Journal of Physical Chemistry C, 2016, 120, 14918-14925.	3.1	16
92	Methyl crotonate hydrogenation over Pt: Effects of support and metal dispersion. Applied Catalysis A: General, 2016, 511, 106-116.	4.3	6
93	TiOx thin films grown on Pd(100) and Pd(111) by chemical vapor deposition. Surface Science, 2016, 649, 80-89.	1.9	12
94	Structural and Energetic Trends of Ethylene Hydrogenation over Transition Metal Surfaces. Journal of Physical Chemistry C, 2016, 120, 995-1003.	3.1	39
95	Insights on proximity effect and multiphoton induced luminescence from gold nanospheres in far field optical microscopy. Applied Physics Letters, 2015, 107, 234101.	3.3	11
96	Revealing local variations in nanoparticle size distributions in supported catalysts: a generic TEM specimen preparation method. Journal of Microscopy, 2015, 260, 125-132.	1.8	8
97	Transient Bimodal Particle Size Distributions during Pt Sintering on Alumina and Silica. Journal of Physical Chemistry C, 2015, 119, 989-996.	3.1	36
98	Size Effects in MgO Cube Dissolution. Langmuir, 2015, 31, 2770-2776.	3.5	49
99	Chemistry of Supported Palladium Nanoparticles during Methane Oxidation. ACS Catalysis, 2015, 5, 2481-2489.	11.2	98
100	NO_x Adsorption on ATiO₃(001) Perovskite Surfaces. Journal of Physical Chemistry C, 2015, 119, 18495-18503.	3.1	11
101	Trends in adsorbate induced core level shifts. Surface Science, 2015, 640, 59-64.	1.9	21
102	Electro-oxidation of water on hematite: Effects of surface termination and oxygen vacancies investigated by first-principles. Surface Science, 2015, 640, 45-49.	1.9	43
103	Methane Oxidation over PdO(101) Revealed by First-Principles Kinetic Modeling. Journal of the American Chemical Society, 2015, 137, 12035-12044.	13.7	104
104	Oxidation at the Subnanometer Scale. Journal of Physical Chemistry C, 2015, 119, 10797-10803.	3.1	14
105	In Situ Plasmonic Sensing of Platinum Model Catalyst Sintering on Different Oxide Supports and in O₂ and NO₂ Atmospheres with Different Concentrations. ACS Catalysis, 2015, 5, 426-432.	11.2	18
106	Selectivity and kinetics of methyl crotonate hydrogenation over Pt/Al₂O₃. Catalysis Science and Technology, 2015, 5, 1716-1730.	4.1	14
107	Effects of non-local exchange on core level shifts for gas-phase and adsorbed molecules. Journal of Chemical Physics, 2014, 141, 034706.	3.0	29
108	Activity of Platinum/Carbon and Palladium/Carbon Catalysts Promoted by Ni₂P in Direct Ethanol Fuel Cells. ChemSusChem, 2014, 7, 3374-3381.	6.8	37

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109	Metalâ€oxide sites for facile methane dissociation. Physica Status Solidi - Rapid Research Letters, 2014, 8, 605-609.	2.4	6
110	CO Adsorption on Clean and Oxidized Pd(111). Journal of Physical Chemistry C, 2014, 118, 1118-1128.	3.1	69
111	Analysis of Porphyrines as Catalysts for Electrochemical Reduction of O₂ and Oxidation of H₂O. Journal of the American Chemical Society, 2014, 136, 1320-1326.	13.7	124
112	Toward a Silverâ€“Alumina Model System for NO_x Reduction Catalysis. Journal of Physical Chemistry C, 2014, 118, 24556-24561.	3.1	3
113	Catalytic hydrogenation of Cî€C and Cî€O in unsaturated fatty acid methyl esters. Catalysis Science and Technology, 2014, 4, 2427-2444.	4.1	52
114	Mechanism for Limiting Thickness of Thin Oxide Films on Aluminum. Physical Review Letters, 2014, 112, 146103.	7.8	74
115	Anchoring of Pt and PtRu to carbon nanofibers studied by density functional theory calculations. Carbon, 2014, 77, 880-885.	10.3	6
116	Intrinsic Ligand Effect Governing the Catalytic Activity of Pd Oxide Thin Films. ACS Catalysis, 2014, 4, 3330-3334.	11.2	79
117	High-Coverage Oxygen-Induced Surface Structures on Ag(111). Journal of Physical Chemistry C, 2014, 118, 15324-15331.	3.1	46
118	Methane oxidation over Pd and Pt studied by DFT and kinetic modeling. Surface Science, 2013, 616, 206-213.	1.9	87
119	Water desorption from nanostructured graphite surfaces. Physical Chemistry Chemical Physics, 2013, 15, 20456.	2.8	16
120	H₂dissociation over Ag/Al₂O₃: the first step in hydrogen assisted selective catalytic reduction of NO_x. Catalysis Science and Technology, 2013, 3, 183-190.	4.1	21
121	Facile NOx interconversion over preoxidized Ag(111). Surface Science, 2013, 617, 167-174.	1.9	5
122	Methane Oxidation Over Pd Supported on Ceriaâ€“Alumina Under Rich/Lean Cycling Conditions. Topics in Catalysis, 2013, 56, 410-415.	2.8	26
123	Efficient hydrogenation over single-site bimetallic RuSn clusters. Physical Chemistry Chemical Physics, 2013, 15, 9694.	2.8	15
124	Dissociative Adsorption of Hydrogen on PdO(101) Studied by HRCLS and DFT. Journal of Physical Chemistry C, 2013, 117, 13510-13519.	3.1	25
125	Generation and oxidation of aerosol deposited PdAg nanoparticles. Surface Science, 2013, 616, 186-191.	1.9	10
126	Mechanism for reversed photoemission core-level shifts of oxidized Ag. Physical Review B, 2012, 85, .	3.2	34

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127	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.	3.1	43
128	Simulated Photoemission Spectra of Hydroxylated MgO(100) at Elevated Temperatures. Journal of Physical Chemistry C, 2012, 116, 3545-3551.	3.1	15
129	Surface composition of clean and oxidized Pd75Ag25(100) from photoelectron spectroscopy and density functional theory calculations. Surface Science, 2012, 606, 1777-1782.	1.9	34
130	Local Catalytic Ignition during CO Oxidation on Lowâ€Index Pt and Pd Surfaces: A Combined PEEM, MS, and DFT Study. Angewandte Chemie - International Edition, 2012, 51, 10041-10044.	13.8	85
131	The Active Phase of Palladium during Methane Oxidation. Journal of Physical Chemistry Letters, 2012, 3, 678-682.	4.6	183
132	The bonding in thiolate protected gold nanoparticles from Au4f photoemission core level shifts. Nanoscale, 2012, 4, 4178.	5.6	16
133	Phase Separation at the Nanoscale: Structural Properties of BaO Segregates on MgO-Based Nanoparticles. Journal of Physical Chemistry C, 2011, 115, 15853-15861.	3.1	26
134	Effect of lattice strain on hydrogen diffusion in Pd: A density functional theory study. Physical Review B, 2011, 84, .	3.2	35
135	CO Oxidation on Technological Pdâ"Al₂O₃Catalysts: Oxidation State and Activity. Journal of Physical Chemistry C, 2011, 115, 1103-1111.	3.1	129
136	The Al50Cp*12 Cluster - A 138-Electron Closed Shell (L = 6) Superatom. European Journal of Inorganic Chemistry, 2011, 2011, 2649-2652.	2.0	41
137	Oxidation and reduction of Pd(100) and aerosol-deposited Pd nanoparticles. Physical Review B, 2011, 83, .	3.2	79
138	Carbonate formation on<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:mi>p</mml:mi><mml:mo>(</mml:mo><mml:mn>4</mml:mn><mml:mo>Ã—</mml:mo><mml:mn>4 Physical Review B, 2011, 84, .	3.2	20
139	Evidence of superatom electronic shells in ligand-stabilized aluminum clusters. Journal of Chemical Physics, 2011, 135, 094701.	3.0	42
140	Exceptionally Active Singleâ€Site Nanocluster Multifunctional Catalysts for Cascade Reactions. ChemCatChem, 2010, 2, 402-406.	3.7	19
141	Photoemission core-level shifts reveal the thiolate-Au(111) interface. Physical Review B, 2010, 82, .	3.2	20
142	Theoretical Characterization of Cyclic Thiolated Copper, Silver, and Gold Clusters. Journal of Physical Chemistry C, 2010, 114, 13571-13576.	3.1	51
143	Oxidation of Small Silver Clusters: A Density Functional Theory Study. Journal of Physical Chemistry C, 2010, 114, 12610-12617.	3.1	55
144	Thiolate-Protected Au₂₅ Superatoms as Building Blocks: Dimers and Crystals. Journal of Physical Chemistry C, 2010, 114, 15986-15994.	3.1	109

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145	Thiolate Induced Reconstruction of Au(111) and Cu(111) Investigated by Density Functional Theory Calculations. Journal of Physical Chemistry C, 2010, 114, 15973-15978.	3.1	38
146	Water Dissociation on MgO/Ag(100): Support Induced Stabilization or Electron Pairing?. Journal of Physical Chemistry C, 2010, 114, 7070-7075.	3.1	34
147	Corrosion Induced Degradation of Pt/C Model Electrodes Measured with Electrochemical Quartz Crystal Microbalance. Journal of the Electrochemical Society, 2010, 157, B592.	2.9	39
148	Experimental and theoretical characterization of NOx species on Ag/Î±-Al2O3. Journal of Molecular Catalysis A, 2009, 314, 102-109.	4.8	22
149	SOx storage and release kinetics for ceria-supported platinum. Applied Catalysis B: Environmental, 2009, 91, 679-682.	20.2	13
150	Low Temperature CO Oxidation over Supported Ultrathin MgO Films. Journal of the American Chemical Society, 2009, 131, 16636-16637.	13.7	121
151	Characterization of Ironâ“Carbonyl-Protected Gold Clusters. Journal of the American Chemical Society, 2009, 131, 12573-12575.	13.7	17
152	First-Principles Studies of NO_xChemistry on Ag_n/Î±-Al₂O₃. Journal of Physical Chemistry C, 2009, 113, 3674-3682.	3.1	35
153	Structure and Bonding in the Ubiquitous Icosahedral Metallic Gold Cluster Au₁₄₄(SR)₆₀. Journal of Physical Chemistry C, 2009, 113, 5035-5038.	3.1	393
154	Regenerable ceria-based SOx traps for sulfur removal in lean exhausts. Applied Catalysis B: Environmental, 2008, 84, 268-276.	20.2	49
155	Identifying surface species by vibrational spectroscopy: Bridging vs monodentate nitrates. Journal of Catalysis, 2008, 255, 127-133.	6.2	52
156	Goldâ“Thiolate Complexes Form a Unique c(4 Ã— 2) Structure on Au(111). Journal of Physical Chemistry C, 2008, 112, 15940-15942.	3.1	125
157	Activation of<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:msub><mml:mi>Al</mml:mi><mml:mn>2</mml:mn></mml:msub><mml:msub><mml:mi mathvariant="normal">O</mml:mi><mml:mn>3</mml:mn></mml:msub></mml:math>by a Long-Ranged Chemical Bond Mechanism. Physical Review Letters, 2008, 100, 116801.	7.8	31
158	On the Structure of Thiolate-Protected Au₂₅. Journal of the American Chemical Society, 2008, 130, 3756-3757.	13.7	682
159	Synthesis, characterization, electronic structure and catalytic performance of bimetallic and trimetallic nanoparticles containing tin. Faraday Discussions, 2008, 138, 301-315.	3.2	62
160	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.	7.1	1,472
161	NO2 dissociation on Ag(111) revisited by theory. Journal of Chemical Physics, 2008, 128, 104704.	3.0	16
162	Ab initiomolecular dynamics calculations of<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:msub><mml:mtext>H</mml:mtext><mml:mn>2</mml:mn></mml:msub><mml:mtext>O</mml:mte BaO(001). Physical Review B, 2008, 77, .	3.2	21

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163	Charging of atoms, clusters, and molecules on metal-supported oxides: A general and long-ranged phenomenon. Physical Review B, 2008, 78, .	3.2	74
164	Vibrational analysis of H<inf>2</inf> and NH<inf>3</inf> adsorption on Pt/SiO<inf>2</inf> and Ir/SiO<inf>2</inf> model sensors. , 2007, , .		1
165	Polymerization at the Alkylthiolateâ^'Au(111) Interface. Journal of Physical Chemistry B, 2007, 111, 3325-3327.	2.6	73
166	Structural, Energetic, and Vibrational Properties of NOxAdsorption on Agn,n= 1â^'8. Journal of Physical Chemistry A, 2007, 111, 6062-6067.	2.5	43
167	Structural and electronic properties of a trimetallic nanoparticle catalyst: Ru5PtSn. Chemical Physics Letters, 2007, 443, 337-341.	2.6	10
168	Methane oxidation over alumina supported platinum investigated by time-resolved in situ XANES spectroscopy. Journal of Catalysis, 2007, 252, 11-17.	6.2	65
169	Divide and Protect:Â Capping Gold Nanoclusters with Molecular Goldâ^'Thiolate Rings. Journal of Physical Chemistry B, 2006, 110, 9927-9931.	2.6	405
170	Mechanism for NO2Charging on Metal Supported MgO. Journal of Physical Chemistry B, 2006, 110, 11977-11981.	2.6	91
171	Theoretical Characterization of Cyclic Thiolated Gold Clusters. Journal of the American Chemical Society, 2006, 128, 10268-10275.	13.7	118
172	Fundamental aspects of NOx adsorption on BaO. Surface Science, 2006, 600, 403-408.	1.9	51
173	Effects of the metal in the adsorption of NO2 on platinum supported BaO films. Surface Science, 2006, 600, L214-L218.	1.9	16
174	Comparison of the bonding inAu8andCu8: A density functional theory study. Physical Review B, 2005, 71, .	3.2	61
175	Toward a Realistic Description of NOxStorage in BaO:Â The Aspect of BaCO3. Journal of Physical Chemistry B, 2005, 109, 9613-9621.	2.6	30
176	The Nature of NOxSpecies on BaO(100):Â An Ab Initio Molecular Dynamics Study. Journal of Physical Chemistry B, 2005, 109, 15410-15416.	2.6	39
177	Vibrational Analysis of H2and D2Adsorption on Pt/SiO2. Journal of Physical Chemistry B, 2005, 109, 9581-9588.	2.6	38
178	Promoting and poisoning effects of Na and Cl coadsorption on CO oxidation over MgO-supported Au nanoparticles. Journal of Catalysis, 2004, 227, 217-226.	6.2	61
179	First Principles Studies of Metal-Oxide Surfaces. Topics in Catalysis, 2004, 28, 59-69.	2.8	41
180	Surface properties of alkaline earth metal oxides. Surface Science, 2004, 554, 262-271.	1.9	90

#	Article	IF	Citations
181	CO bonded to platinum: effects of semi-core polarization. Surface Science, 2004, 559, 214-222.	1.9	11
182	Vibrational study of ammonia adsorption on Pt/SiO2. Applied Surface Science, 2004, 235, 487-500.	6.1	60
183	NOx storage on BaO: theory and experiment. Catalysis Today, 2004, 96, 71-78.	4.4	91
184	Characterization of NOxSpecies Adsorbed on BaO:Â Experiment and Theory. Journal of Physical Chemistry B, 2004, 108, 3523-3530.	2.6	73
185	CO bonded to platinum: effects of semi-core polarization. Surface Science, 2004, 559, 214-214.	1.9	1
186	Pt and Pt2 on MgO(100) and BaO(100): structure, bonding, and chemical properties. Journal of Chemical Physics, 2003, 119, 3896-3904.	3.0	41
187	CO-Induced Modification of the Metal/MgO(100) Interaction. Journal of Physical Chemistry B, 2003, 107, 12239-12243.	2.6	36
188	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.	2.6	38
189	Assessing the validity of theoretical results. European Physical Journal D, 2001, 16, 29-32.	1.3	8
190	Density functional theory approach to thiols and disulfides on gold: Au(111) surface and clusters. International Journal of Quantum Chemistry, 2000, 80, 598-608.	2.0	116
191	Gold and platinum microclusters and their anions: comparison of structural and electronic properties. Chemical Physics, 2000, 262, 1-14.	1.9	149
192	Thiols and Disulfides on the Au(111) Surface:Â The Headgroupâ^'Gold Interaction. Journal of the American Chemical Society, 2000, 122, 3839-3842.	13.7	591
193	Molecular dynamics simulation of metal cluster cooling and heating in noble gas atmosphere. Scripta Materialia, 1999, 12, 281-286.	0.5	6
194	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.	3.0	37
195	Structural, electronic, and vibrational properties of neutral and chargedNbnâ€,(n=8,9,10)clusters. Physical Review A, 1998, 58, 4630-4636.	2.5	44
196	Noble gas temperature control of metal clusters: A molecular dynamics study. Journal of Chemical Physics, 1997, 107, 3071-3079.	3.0	71
197	Geometric and electronic properties of small vanadium clusters: A density functional study. Journal of Chemical Physics, 1997, 107, 10620-10625.	3.0	67
198	Theoretical study of chemisorption on niobium clusters: carbon monoxide and oxygen. Zeitschrift FÃ¼r Physik D-Atoms Molecules and Clusters, 1997, 40, 206-209.	1.0	13

#	Article	IF	Citations
199	Hydrogen induced melting of Palladium clusters. Zeitschrift FÃ¼r Physik D-Atoms Molecules and Clusters, 1997, 40, 469-471.	1.0	9
200	Does hydrogen pre-melt palladium clusters?. Chemical Physics Letters, 1997, 264, 39-43.	2.6	17
201	Theoretical study of (CO)n chemisorption on Pt and Pt3: structural, electronic and vibrational properties. Chemical Physics Letters, 1997, 269, 385-390.	2.6	14
202	Theoretical study of chemisorption on niobium clusters: carbon monoxide and oxygen. , 1997, , 206-209.		0
203	ELECTRONIC STRUCTURE OF ASSEMBLED CLUSTERS WITHIN THE STABILIZED JELLIUM MODEL. Surface Review and Letters, 1996, 03, 1001-1006.	1.1	0
204	Analysis of the odd-even alternation in simple metal clusters. Zeitschrift FÃ¼r Physik D-Atoms Molecules and Clusters, 1996, 36, 153-157.	1.0	18
205	CO on copper clusters: Orbital symmetry rules. Physical Review B, 1996, 53, 16644-16651.	3.2	38
206	Investigation of niobium clusters: Bare and CO-adsorption. Physical Review B, 1996, 54, 1549-1552.	3.2	45
207	CHEMISORPTION OF O2 AND CO ON COPPER CLUSTERS. Surface Review and Letters, 1996, 03, 687-693.	1.1	8
208	Reactivity of small transition-metal clusters with CO. , 1995, , .		1
209	Harmonic heat flow in anisotropic thin films. Journal of Applied Physics, 1995, 78, 6408-6413.	2.5	11
210	Chemisorption of molecular oxygen on copper clusters studied by jellium and MO-LCAO models. Scripta Materialia, 1995, 5, 193-206.	0.5	5
211	Harmonic heat flow in isotropic layered systems and its use for thin film thermal conductivity measurements. Journal of Applied Physics, 1994, 75, 1914-1922.	2.5	85
212	A jellium approach to the chemisorption of molecular oxygen on copper clusters. Chemical Physics Letters, 1994, 227, 149-156.	2.6	15
213	Chemisorption of molecular oxygen on small copper clusters and the Cu(100) surface. Computational Materials Science, 1994, 2, 607-614.	3.0	5
214	Electronic Structure Calculations of Pure and Oxidized Copper Clusters Using Jellium and MO - LCAO Models. Materials Research Society Symposia Proceedings, 1994, 351, 15.	0.1	0
215	<title>Photothermal measurement of thermal conductivity of optical coatings</title>. , 1992, , .		4
216	<title>Thermal transport studies of diamond thin films</title>. , 1992, , .		0