

Henrik Grønbeck

List of Publications by Year in descending order

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222
docs citations

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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. | 7.1 | 1,472 |
| 2 | On the Structure of Thiolate-Protected Au ₂₅ . Journal of the American Chemical Society, 2008, 130, 3756-3757. | 13.7 | 682 |
| 3 | Thiols and Disulfides on the Au(111) Surface: The Headgroup-Gold Interaction. Journal of the American Chemical Society, 2000, 122, 3839-3842. | 13.7 | 591 |
| 4 | Divide and Protect: Capping Gold Nanoclusters with Molecular Gold-Thiolate Rings. Journal of Physical Chemistry B, 2006, 110, 9927-9931. | 2.6 | 405 |
| 5 | Structure and Bonding in the Ubiquitous Icosahedral Metallic Gold Cluster Au ₁₄₄ (SR) ₆₀ . Journal of Physical Chemistry C, 2009, 113, 5035-5038. | 3.1 | 393 |
| 6 | The Active Phase of Palladium during Methane Oxidation. Journal of Physical Chemistry Letters, 2012, 3, 678-682. | 4.6 | 183 |
| 7 | Gold and platinum microclusters and their anions: comparison of structural and electronic properties. Chemical Physics, 2000, 262, 1-14. | 1.9 | 149 |
| 8 | CO Oxidation on Technological Pd ₂ O ₃ Catalysts: Oxidation State and Activity. Journal of Physical Chemistry C, 2011, 115, 1103-1111. | 3.1 | 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. | 3.1 | 125 |
| 10 | Analysis of Porphyrines as Catalysts for Electrochemical Reduction of O ₂ and Oxidation of H ₂ O. Journal of the American Chemical Society, 2014, 136, 1320-1326. | 13.7 | 124 |
| 11 | Low Temperature CO Oxidation over Supported Ultrathin MgO Films. Journal of the American Chemical Society, 2009, 131, 16636-16637. | 13.7 | 121 |
| 12 | Theoretical Characterization of Cyclic Thiolated Gold Clusters. Journal of the American Chemical Society, 2006, 128, 10268-10275. | 13.7 | 118 |
| 13 | A Complete Multisite Reaction Mechanism for Low-Temperature NH ₃ -SCR over Cu-CHA. ACS Catalysis, 2020, 10, 5646-5656. | 11.2 | 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. | 2.0 | 116 |
| 15 | Thiolate-Protected Au ₂₅ Superatoms as Building Blocks: Dimers and Crystals. Journal of Physical Chemistry C, 2010, 114, 15986-15994. | 3.1 | 109 |
| 16 | Methane Oxidation over PdO(101) Revealed by First-Principles Kinetic Modeling. Journal of the American Chemical Society, 2015, 137, 12035-12044. | 13.7 | 104 |
| 17 | Influence of atomic site-specific strain on catalytic activity of supported nanoparticles. Nature Communications, 2018, 9, 2722. | 12.8 | 102 |
| 18 | Chemistry of Supported Palladium Nanoparticles during Methane Oxidation. ACS Catalysis, 2015, 5, 2481-2489. | 11.2 | 98 |

| # | ARTICLE | IF | CITATIONS |
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| 19 | NOx storage on BaO: theory and experiment. <i>Catalysis Today</i> , 2004, 96, 71-78. | 4.4 | 91 |
| 20 | Mechanism for NO ₂ Charging on Metal Supported MgO. <i>Journal of Physical Chemistry B</i> , 2006, 110, 11977-11981. | 2.6 | 91 |
| 21 | Activation of oxygen on (NH ₃ Cu NH ₃) ⁺ in NH ₃ -SCR over Cu-CHA. <i>Journal of Catalysis</i> , 2018, 358, 179-186. | 6.2 | 91 |
| 22 | Surface properties of alkaline earth metal oxides. <i>Surface Science</i> , 2004, 554, 262-271. | 1.9 | 90 |
| 23 | First-Principles Microkinetic Modeling of Methane Oxidation over Pd(100) and Pd(111). <i>ACS Catalysis</i> , 2016, 6, 6730-6738. | 11.2 | 88 |
| 24 | Methane oxidation over Pd and Pt studied by DFT and kinetic modeling. <i>Surface Science</i> , 2013, 616, 206-213. | 1.9 | 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. | 2.5 | 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. | 13.8 | 85 |
| 27 | Oxidation and reduction of Pd(100) and aerosol-deposited Pd nanoparticles. <i>Physical Review B</i> , 2011, 83, . | 3.2 | 79 |
| 28 | Intrinsic Ligand Effect Governing the Catalytic Activity of Pd Oxide Thin Films. <i>ACS Catalysis</i> , 2014, 4, 3330-3334. | 11.2 | 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, . | 3.2 | 74 |
| 30 | Mechanism for Limiting Thickness of Thin Oxide Films on Aluminum. <i>Physical Review Letters</i> , 2014, 112, 146103. | 7.8 | 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. | 11.2 | 74 |
| 32 | Characterization of NO _x Species Adsorbed on BaO: Experiment and Theory. <i>Journal of Physical Chemistry B</i> , 2004, 108, 3523-3530. | 2.6 | 73 |
| 33 | Polymerization at the Alkylthiolate-Au(111) Interface. <i>Journal of Physical Chemistry B</i> , 2007, 111, 3325-3327. | 2.6 | 73 |
| 34 | Noble gas temperature control of metal clusters: A molecular dynamics study. <i>Journal of Chemical Physics</i> , 1997, 107, 3071-3079. | 3.0 | 71 |
| 35 | Adsorbate Entropies with Complete Potential Energy Sampling in Microkinetic Modeling. <i>Journal of Physical Chemistry C</i> , 2017, 121, 7199-7207. | 3.1 | 70 |
| 36 | Steps Control the Dissociation of CO ₂ on Cu(100). <i>Journal of the American Chemical Society</i> , 2018, 140, 12974-12979. | 13.7 | 70 |

| # | ARTICLE | IF | CITATIONS |
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| 37 | CO Adsorption on Clean and Oxidized Pd(111). <i>Journal of Physical Chemistry C</i> , 2014, 118, 1118-1128. | 3.1 | 69 |
| 38 | Geometric and electronic properties of small vanadium clusters: A density functional study. <i>Journal of Chemical Physics</i> , 1997, 107, 10620-10625. | 3.0 | 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. | 6.2 | 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. | 13.7 | 63 |
| 41 | Synthesis, characterization, electronic structure and catalytic performance of bimetallic and trimetallic nanoparticles containing tin. <i>Faraday Discussions</i> , 2008, 138, 301-315. | 3.2 | 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. | 6.2 | 61 |
| 43 | Comparison of the bonding in Au ₈ and Cu ₈ : A density functional theory study. <i>Physical Review B</i> , 2005, 71, . | 3.2 | 61 |
| 44 | Real-time imaging of Na ⁺ reversible intercalation in Janus-graphene stacks for battery applications. <i>Science Advances</i> , 2021, 7, . | 10.3 | 61 |
| 45 | Vibrational study of ammonia adsorption on Pt/SiO ₂ . <i>Applied Surface Science</i> , 2004, 235, 487-500. | 6.1 | 60 |
| 46 | Interpretation of NH ₃ -TPD Profiles from Cu-CHA Using First-Principles Calculations. <i>Topics in Catalysis</i> , 2019, 62, 93-99. | 2.8 | 60 |
| 47 | Metal dimer sites in ZSM-5 zeolite for methane-to-methanol conversion from first-principles kinetic modelling: is the [Cu-O-Cu] ²⁺ motif relevant for Ni, Co, Fe, Ag, and Au?. <i>Catalysis Science and Technology</i> , 2017, 7, 1470-1477. | 4.1 | 56 |
| 48 | Oxidation of Small Silver Clusters: A Density Functional Theory Study. <i>Journal of Physical Chemistry C</i> , 2010, 114, 12610-12617. | 3.1 | 55 |
| 49 | Identifying surface species by vibrational spectroscopy: Bridging vs monodentate nitrates. <i>Journal of Catalysis</i> , 2008, 255, 127-133. | 6.2 | 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. | 4.1 | 52 |
| 51 | Fundamental aspects of NO _x adsorption on BaO. <i>Surface Science</i> , 2006, 600, 403-408. | 1.9 | 51 |
| 52 | Theoretical Characterization of Cyclic Thiolated Copper, Silver, and Gold Clusters. <i>Journal of Physical Chemistry C</i> , 2010, 114, 13571-13576. | 3.1 | 51 |
| 53 | On the Reaction Mechanism of Direct H ₂ O ₂ Formation over Pd Catalysts. <i>ACS Catalysis</i> , 2021, 11, 2735-2745. | 11.2 | 50 |
| 54 | Regenerable ceria-based SO _x traps for sulfur removal in lean exhausts. <i>Applied Catalysis B: Environmental</i> , 2008, 84, 268-276. | 20.2 | 49 |

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| 55 | Size Effects in MgO Cube Dissolution. <i>Langmuir</i> , 2015, 31, 2770-2776. | 3.5 | 49 |
| 56 | The Site Assembly Determines Catalytic Activity of Nanoparticles. <i>Angewandte Chemie - International Edition</i> , 2018, 57, 5086-5089. | 13.8 | 49 |
| 57 | Methane oxidation over Pd/Al ₂ O ₃ under rich/lean cycling followed by operando XAFS and modulation excitation spectroscopy. <i>Journal of Catalysis</i> , 2017, 356, 237-245. | 6.2 | 48 |
| 58 | Effect of Al-distribution on oxygen activation over Cu-CHA. <i>Catalysis Science and Technology</i> , 2018, 8, 2131-2136. | 4.1 | 47 |
| 59 | High-Coverage Oxygen-Induced Surface Structures on Ag(111). <i>Journal of Physical Chemistry C</i> , 2014, 118, 15324-15331. | 3.1 | 46 |
| 60 | Investigation of niobium clusters: Bare and CO-adsorption. <i>Physical Review B</i> , 1996, 54, 1549-1552. | 3.2 | 45 |
| 61 | Structural, electronic, and vibrational properties of neutral and charged Nb _n (n=8,9,10) clusters. <i>Physical Review A</i> , 1998, 58, 4630-4636. | 2.5 | 44 |
| 62 | Structural, Energetic, and Vibrational Properties of NO _x Adsorption on Ag _n , n= 1~8. <i>Journal of Physical Chemistry A</i> , 2007, 111, 6062-6067. | 2.5 | 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. | 3.1 | 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. | 1.9 | 43 |
| 65 | Kinetic Regimes in Ethylene Hydrogenation over Transition-Metal Surfaces. <i>ACS Catalysis</i> , 2016, 6, 3277-3286. | 11.2 | 43 |
| 66 | Evidence of superatom electronic shells in ligand-stabilized aluminum clusters. <i>Journal of Chemical Physics</i> , 2011, 135, 094701. | 3.0 | 42 |
| 67 | Pt and Pt ₂ on MgO(100) and BaO(100): structure, bonding, and chemical properties. <i>Journal of Chemical Physics</i> , 2003, 119, 3896-3904. | 3.0 | 41 |
| 68 | First Principles Studies of Metal-Oxide Surfaces. <i>Topics in Catalysis</i> , 2004, 28, 59-69. | 2.8 | 41 |
| 69 | The Al ₅₀ Cp* ₁₂ Cluster - A 138-Electron Closed Shell (L = 6) Superatom. <i>European Journal of Inorganic Chemistry</i> , 2011, 2011, 2649-2652. | 2.0 | 41 |
| 70 | A comparative test of different density functionals for calculations of NH ₃ -SCR over Cu-Chabazite. <i>Physical Chemistry Chemical Physics</i> , 2019, 21, 10923-10930. | 2.8 | 40 |
| 71 | The Nature of NO _x Species on BaO(100): An Ab Initio Molecular Dynamics Study. <i>Journal of Physical Chemistry B</i> , 2005, 109, 15410-15416. | 2.6 | 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. | 2.9 | 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. | 3.1 | 39 |
| 74 | High Specific and Mass Activity for the Oxygen Reduction Reaction for Thin Film Catalysts of Sputtered Pt ₃ Y. Advanced Materials Interfaces, 2017, 4, 1700311. | 3.7 | 39 |
| 75 | CO on copper clusters: Orbital symmetry rules. Physical Review B, 1996, 53, 16644-16651. | 3.2 | 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. | 2.6 | 38 |
| 77 | Vibrational Analysis of H ₂ and D ₂ Adsorption on Pt/SiO ₂ . Journal of Physical Chemistry B, 2005, 109, 9581-9588. | 2.6 | 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. | 3.1 | 38 |
| 79 | Understanding the Intrinsic Surface Reactivity of Single-Layer and Multilayer PdO(101) on Pd(100). ACS Catalysis, 2018, 8, 8553-8567. | 11.2 | 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. | 3.0 | 37 |
| 81 | Activity of Platinum/Carbon and Palladium/Carbon Catalysts Promoted by Ni ₂ P in Direct Ethanol Fuel Cells. ChemSusChem, 2014, 7, 3374-3381. | 6.8 | 37 |
| 82 | CO-Induced Modification of the Metal/MgO(100) Interaction. Journal of Physical Chemistry B, 2003, 107, 12239-12243. | 2.6 | 36 |
| 83 | Transient Bimodal Particle Size Distributions during Pt Sintering on Alumina and Silica. Journal of Physical Chemistry C, 2015, 119, 989-996. | 3.1 | 36 |
| 84 | Strain Dependent Light-off Temperature in Catalysis Revealed by Planar Laser-Induced Fluorescence. ACS Catalysis, 2017, 7, 110-114. | 11.2 | 36 |
| 85 | First-Principles Studies of NO _x Chemistry on Ag _n /Al ₂ O ₃ . Journal of Physical Chemistry C, 2009, 113, 3674-3682. | 3.1 | 35 |
| 86 | Effect of lattice strain on hydrogen diffusion in Pd: A density functional theory study. Physical Review B, 2011, 84, . | 3.2 | 35 |
| 87 | Water Dissociation on MgO/Ag(100): Support Induced Stabilization or Electron Pairing?. Journal of Physical Chemistry C, 2010, 114, 7070-7075. | 3.1 | 34 |
| 88 | Mechanism for reversed photoemission core-level shifts of oxidized Ag. Physical Review B, 2012, 85, . | 3.2 | 34 |
| 89 | Surface composition of clean and oxidized Pd ₇₅ Ag ₂₅ (100) from photoelectron spectroscopy and density functional theory calculations. Surface Science, 2012, 606, 1777-1782. | 1.9 | 34 |
| 90 | Perspectives on Computational Catalysis for Metal Nanoparticles. ACS Catalysis, 2019, 9, 8872-8881. | 11.2 | 34 |

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| 91 | Mechanism for Solid-State Ion Exchange of Cu ⁺ into Zeolites. <i>Journal of Physical Chemistry C</i> , 2016, 120, 29182-29189. | 3.1 | 33 |
| 92 | Catalysis at the Rim: A Mechanism for Low Temperature CO Oxidation over Pt ₃ Sn. <i>ACS Catalysis</i> , 2017, 7, 7431-7441. | 11.2 | 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. | 3.1 | 32 |
| 94 | Activation of Al_2O_3 by a Long-Ranged Chemical Bond Mechanism. <i>Physical Review Letters</i> , 2008, 100, 116801. | 7.8 | 31 |
| 95 | Reversed Hysteresis during CO Oxidation over Pd ₇₅ Ag ₂₅ (100). <i>ACS Catalysis</i> , 2016, 6, 4154-4161. | 11.2 | 31 |
| 96 | Visualizing catalyst heterogeneity by a multifrequential oscillating reaction. <i>Nature Communications</i> , 2018, 9, 600. | 12.8 | 31 |
| 97 | Tight-Binding Approximation-Enhanced Global Optimization. <i>Journal of Chemical Theory and Computation</i> , 2018, 14, 2797-2807. | 5.3 | 31 |
| 98 | Toward a Realistic Description of NO _x Storage in BaO: The Aspect of BaCO ₃ . <i>Journal of Physical Chemistry B</i> , 2005, 109, 9613-9621. | 2.6 | 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. | 3.0 | 29 |
| 100 | First Principles Calculations of Palladium Nanoparticle XANES Spectra. <i>Topics in Catalysis</i> , 2017, 60, 283-288. | 2.8 | 28 |
| 101 | The Role of H ⁻ and Cu ⁺ -Sites for N ₂ O Formation during NH ₃ -SCR over Cu-CHA. <i>Journal of Physical Chemistry C</i> , 2021, 125, 4595-4601. | 3.1 | 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. | 3.1 | 27 |
| 103 | Monte Carlo Potential Energy Sampling for Molecular Entropy in Zeolites. <i>Journal of Physical Chemistry C</i> , 2018, 122, 20351-20357. | 3.1 | 27 |
| 104 | Interplay between CO Disproportionation and Oxidation: On the Origin of the CO Reaction Onset on Atomic Layer Deposition-Grown Pt/ZrO ₂ Model Catalysts. <i>ACS Catalysis</i> , 2021, 11, 208-214. | 11.2 | 27 |
| 105 | On the signatures of oxygen vacancies in O1s core level shifts. <i>Surface Science</i> , 2021, 705, 121761. | 1.9 | 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. | 3.1 | 26 |
| 107 | Methane Oxidation Over Pd Supported on Ceria-Alumina Under Rich/Lean Cycling Conditions. <i>Topics in Catalysis</i> , 2013, 56, 410-415. | 2.8 | 26 |
| 108 | 2D-3D structural transition in sub-nanometer Pt _N clusters supported on CeO ₂ (111). <i>Physical Chemistry Chemical Physics</i> , 2017, 19, 17845-17855. | 2.8 | 26 |

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| 109 | MonteCoffee: A programmable kinetic Monte Carlo framework. Journal of Chemical Physics, 2018, 149, 114101. | 3.0 | 26 |
| 110 | Dissociative Adsorption of Hydrogen on PdO(101) Studied by HRCLS and DFT. Journal of Physical Chemistry C, 2013, 117, 13510-13519. | 3.1 | 25 |
| 111 | First-Principles Microkinetic Model for Low-Temperature NH ₃ -Assisted Selective Catalytic Reduction of NO over Cu-CHA. ACS Catalysis, 2021, 11, 14395-14407. | 11.2 | 25 |
| 112 | Tunable Ti ³⁺ -Mediated Charge Carrier Dynamics of Atomic Layer Deposition-Grown Amorphous TiO ₂ . Journal of Physical Chemistry C, 2022, 126, 4542-4554. | 3.1 | 25 |
| 113 | A Chemical View on X-ray Photoelectron Spectroscopy: the ESCA Molecule and Surface to Bulk XPS Shifts. ChemPhysChem, 2018, 19, 169-174. | 2.1 | 24 |
| 114 | CO ₂ adsorption on hydroxylated In ₂ O ₃ (110). Physical Chemistry Chemical Physics, 2019, 21, 21698-21708. | 2.8 | 23 |
| 115 | Experimental and theoretical characterization of NO _x species on Ag/Al ₂ O ₃ . Journal of Molecular Catalysis A, 2009, 314, 102-109. | 4.8 | 22 |
| 116 | Thermal Stability of Single-Crystalline IrO ₂ (110) Layers: Spectroscopic and Adsorption Studies. Journal of Physical Chemistry C, 2020, 124, 15324-15336. | 3.1 | 22 |
| 117 | Resolving multifrequential oscillations and nanoscale interfacet communication in single-particle catalysis. Science, 2021, 372, 1314-1318. | 12.6 | 22 |
| 118 | <i>Ab initio</i> molecular dynamics calculations of H_2O on BaO(001). Physical Review B, 2008, 77, . | 3.2 | 21 |
| 119 | H ₂ dissociation over Ag/Al ₂ O ₃ : the first step in hydrogen assisted selective catalytic reduction of NO _x . Catalysis Science and Technology, 2013, 3, 183-190. | 4.1 | 21 |
| 120 | Trends in adsorbate induced core level shifts. Surface Science, 2015, 640, 59-64. | 1.9 | 21 |
| 121 | Adsorption of NO on Fe ₃ O ₄ (111). Chemical Physics Letters, 2018, 693, 84-87. | 2.6 | 21 |
| 122 | Hydrogen adsorption on In ₂ O ₃ (111) and In ₂ O ₃ (110). Physical Chemistry Chemical Physics, 2020, 22, 16193-16202. | 2.8 | 21 |
| 123 | Photoemission core-level shifts reveal the thiolate-Au(111) interface. Physical Review B, 2010, 82, . | 3.2 | 20 |
| 124 | Carbonate formation on $p(4\sqrt{3} \times \sqrt{3})$. Physical Review B, 2011, 84, . | 3.2 | 20 |
| 125 | Exceptionally Active Single-Site Nanocluster Multifunctional Catalysts for Cascade Reactions. ChemCatChem, 2010, 2, 402-406. | 3.7 | 19 |
| 126 | A First-Principles-Based Microkinetic Study of CO ₂ Reduction to CH ₃ OH over In ₂ O ₃ (110). ACS Catalysis, 2021, 11, 9996-10006. | 11.2 | 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 ₂ and NO ₂ Atmospheres with Different Concentrations. ACS Catalysis, 2015, 5, 426-432. | 11.2 | 18 |
| 129 | Plasmonic Nanospectroscopy of Platinum Catalyst Nanoparticle Sintering in a Mesoporous Alumina Support. ACS Nano, 2016, 10, 5063-5069. | 14.6 | 18 |
| 130 | Thin water films and particle morphology evolution in nanocrystalline MgO. Journal of the American Ceramic Society, 2018, 101, 4994-5003. | 3.8 | 18 |
| 131 | Surface-Structure Libraries: Multifrequential Oscillations in Catalytic Hydrogen Oxidation on Rhodium. Journal of Physical Chemistry C, 2019, 123, 4217-4227. | 3.1 | 18 |
| 132 | Does hydrogen pre-melt palladium clusters?. Chemical Physics Letters, 1997, 264, 39-43. | 2.6 | 17 |
| 133 | Characterization of Iron-Carbonyl-Protected Gold Clusters. Journal of the American Chemical Society, 2009, 131, 12573-12575. | 13.7 | 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. | 4.1 | 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. | 1.9 | 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. | 3.1 | 17 |
| 137 | Effects of the metal in the adsorption of NO ₂ on platinum supported BaO films. Surface Science, 2006, 600, L214-L218. | 1.9 | 16 |
| 138 | NO ₂ dissociation on Ag(111) revisited by theory. Journal of Chemical Physics, 2008, 128, 104704. | 3.0 | 16 |
| 139 | The bonding in thiolate protected gold nanoparticles from Au4f photoemission core level shifts. Nanoscale, 2012, 4, 4178. | 5.6 | 16 |
| 140 | Water desorption from nanostructured graphite surfaces. Physical Chemistry Chemical Physics, 2013, 15, 20456. | 2.8 | 16 |
| 141 | Tuning the Reactivity of Ultrathin Oxides: NO Adsorption on Monolayer FeO(111). Angewandte Chemie - International Edition, 2016, 55, 9267-9271. | 13.8 | 16 |
| 142 | Pt Nanoparticle Sintering and Redispersion on a Heterogeneous Nanostructured Support. Journal of Physical Chemistry C, 2016, 120, 14918-14925. | 3.1 | 16 |
| 143 | Unraveling the Surface Chemistry and Structure in Highly Active Sputtered Pt ₃ Y Catalyst Films for the Oxygen Reduction Reaction. ACS Applied Materials & Interfaces, 2020, 12, 4454-4462. | 8.0 | 16 |
| 144 | A jellium approach to the chemisorption of molecular oxygen on copper clusters. Chemical Physics Letters, 1994, 227, 149-156. | 2.6 | 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. | 3.1 | 15 |
| 146 | Efficient hydrogenation over single-site bimetallic RuSn clusters. Physical Chemistry Chemical Physics, 2013, 15, 9694. | 2.8 | 15 |
| 147 | Cluster Size Effects in Ethylene Hydrogenation over Palladium. Journal of Physical Chemistry C, 2017, 121, 10870-10875. | 3.1 | 15 |
| 148 | Revealing Carbon Phenomena at Palladium Nanoparticles by Analyzing the Work Function. Journal of Physical Chemistry C, 2019, 123, 4360-4370. | 3.1 | 15 |
| 149 | Theoretical study of (CO) _n chemisorption on Pt and Pt ₃ : structural, electronic and vibrational properties. Chemical Physics Letters, 1997, 269, 385-390. | 2.6 | 14 |
| 150 | Oxidation at the Subnanometer Scale. Journal of Physical Chemistry C, 2015, 119, 10797-10803. | 3.1 | 14 |
| 151 | Selectivity and kinetics of methyl crotonate hydrogenation over Pt/Al ₂ O ₃ . Catalysis Science and Technology, 2015, 5, 1716-1730. | 4.1 | 14 |
| 152 | Connection between macroscopic kinetic measurables and the degree of rate control. Catalysis Science and Technology, 2017, 7, 4034-4040. | 4.1 | 14 |
| 153 | Fuel Cell Measurements with Cathode Catalysts of Sputtered Pt ₃ Y Thin Films. ChemSusChem, 2018, 11, 1438-1445. | 6.8 | 14 |
| 154 | Oxygen step-response experiments for methane oxidation over Pd/Al ₂ O ₃ : An in situ XAFS study. Catalysis Communications, 2018, 109, 24-27. | 3.3 | 14 |
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