Sergey M Kozlov

List of Publications by Year
in descending order

59 papers	4,123 citations	117619 34 h-index	133244 59 g-index
61 all docs	61 docs citations	61 times ranked	5894 citing authors

#	Article	IF	Citations
1	Counting electrons on supported nanoparticles. Nature Materials, 2016, 15, 284-288.	27.5	469
2	High-valence metals improve oxygen evolution reaction performance by modulating 3d metal oxidation cycle energetics. Nature Catalysis, 2020, 3, 985-992.	34.4	390
3	Bulk Properties of Transition Metals: A Challenge for the Design of Universal Density Functionals. Journal of Chemical Theory and Computation, 2014, 10, 3832-3839.	5.3	245
4	Establishing the Accuracy of Broadly Used Density Functionals in Describing Bulk Properties of Transition Metals. Journal of Chemical Theory and Computation, 2013, 9, 1631-1640.	5.3	184
5	Solution processable metalâ€“organic frameworks for mixed matrix membranes using porous liquids. Nature Materials, 2020, 19, 1346-1353.	27.5	181
6	Graphene on Ni(111): Coexistence of Different Surface Structures. Journal of Physical Chemistry Letters, 2011, 2, 759-764.	4.6	158
7	The role of metal/oxide interfaces for long-range metal particle activation during CO oxidation. Nature Materials, 2018, 17, 519-522.	27.5	136
8	Bonding Mechanisms of Graphene on Metal Surfaces. Journal of Physical Chemistry C, 2012, 116, 7360-7366.	3.1	133
9	Water Chemistry on Model Ceria and Pt/Ceria Catalysts. Journal of Physical Chemistry C, 2012, 116, 12103-12113.	3.1	108
10	Quantum-Dot-Derived Catalysts for CO2 Reduction Reaction. Joule, 2019, 3, 1703-1718.	24.0	106
11	Doping-Induced Anisotropic Self-Assembly of Silver Icosahedra in [Pt₂Ag₂₃Cl₇(PPh₃)₁₀] Nanoclusters. Journal of the American Chemical Society, 2017, 139, 1053-1056.	13.7	98
12	In-operando elucidation of bimetallic CoNi nanoparticles during high-temperature CH4/CO2 reaction. Applied Catalysis B: Environmental, 2017, 213, 177-189.	20.2	88
13	Turning a Methanation Co Catalyst into an Inâ€“Co Methanol Producer. ACS Catalysis, 2019, 9, 6910-6918.	11.2	88
14	Bandgap Engineering of Graphene by Physisorbed Adsorbates. Advanced Materials, 2011, 23, 2638-2643.	21.0	80
15	Growth and electronic structure of nitrogen-doped graphene on Ni(111). Physical Review B, 2012, 86, .	3.2	77
16	Tailoring the Crystal Structure of Nanoclusters Unveiled High Photoluminescence via Ion Pairing. Chemistry of Materials, 2018, 30, 2719-2725.	6.7	76
17	Role of Oxidized Mo Species on the Active Surface of Niâ€“Mo Electrocatalysts for Hydrogen Evolution under Alkaline Conditions. ACS Catalysis, 2020, 10, 12858-12866.	11.2	75
18	How Absorbed Hydrogen Affects the Catalytic Activity of Transition Metals. Angewandte Chemie - International Edition, 2014, 53, 13371-13375.	13.8	73

#	Article	IF	Citations
19	How to determine accurate chemical ordering in several nanometer large bimetallic crystallites from electronic structure calculations. Chemical Science, 2015, 6, 3868-3880.	7.4	70
20	On the interaction of polycyclic aromatic compounds with graphene. Carbon, 2012, 50, 2482-2492.	10.3	66
21	Direct versus ligand-exchange synthesis of [PtAg₂₈(BDT)₁₂(TPP)₄]^{4â^’}nanoclusters: effect of a single-atom dopant on the optoelectronic and chemical properties. Nanoscale, 2017, 9, 9529-9536.	5.6	62
22	Formation of One-Dimensional Electronic States along the Step Edges of CeO₂(111). ACS Nano, 2012, 6, 1126-1133.	14.6	61
23	Atomic Pd-promoted ZnZrO solid solution catalyst for CO2 hydrogenation to methanol. Applied Catalysis B: Environmental, 2022, 304, 120994.	20.2	59
24	Theoretical assessment of graphene-metal contacts. Journal of Chemical Physics, 2013, 138, 244701.	3.0	58
25	Constructing Bridges between Computational Tools in Heterogeneous and Homogeneous Catalysis. ACS Catalysis, 2018, 8, 5637-5656.	11.2	58
26	Tandem Conversion of CO₂ to Valuable Hydrocarbons in Highly Concentrated Potassium Iron Catalysts. ChemCatChem, 2019, 11, 2879-2886.	3.7	57
27	Stabilization of Small Platinum Nanoparticles on Ptâ€“CeO₂Thin Film Electrocatalysts During Methanol Oxidation. Journal of Physical Chemistry C, 2016, 120, 19723-19736.	3.1	50
28	Surface composition changes of CuNi-ZrO2 during methane decomposition: An operando NAP-XPS and density functional study. Catalysis Today, 2017, 283, 134-143.	4.4	48
29	Effect of MgO(100) support on structure and properties of Pd and Pt nanoparticles with 49-155 atoms. Journal of Chemical Physics, 2013, 139, 084701.	3.0	41
30	Effects of electron transfer in model catalysts composed of Pt nanoparticles on CeO2(1 1 1) surface. Journal of Catalysis, 2016, 344, 507-514.	6.2	41
31	Geometric Arrangement of Components in Bimetallic PdZn/Pd(111) Surfaces Modified by CO Adsorption: A Combined Study by Density Functional Calculations, Polarization-Modulated Infrared Reflection Absorption Spectroscopy, and Temperature-Programmed Desorption. Journal of Physical Chemistry C, 2012, 116, 18768-18778.	3.1	40
32	Efficient electrochemical transformation of CO₂ to C₂/C₃ chemicals on benzimidazole-functionalized copper surfaces. Chemical Communications, 2018, 54, 11324-11327.	4.1	39
33	Absolute Surface Step Energies: Accurate Theoretical Methods Applied to Ceria Nanoislands. Journal of Physical Chemistry Letters, 2012, 3, 1956-1961.	4.6	38
34	Insights from methane decomposition on nanostructured palladium. Journal of Catalysis, 2016, 337, 111-121.	6.2	38
35	Electronic-structure-based material descriptors: (in)dependence on self-interaction and Hartreeâ€“Fock exchange. Chemical Communications, 2015, 51, 5602-5605.	4.1	34
36	Oxygen vacancies in self-assemblies of ceria nanoparticles. Journal of Materials Chemistry A, 2014, 2, 18329-18338.	10.3	33

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37	O vacancies on steps on the CeO2(111) surface. Physical Chemistry Chemical Physics, 2014, 16, 7823.	2.8	33
38	Adsorbed and Subsurface Absorbed Hydrogen Atoms on Bare and MgO(100)-Supported Pd and Pt Nanoparticles. Journal of Physical Chemistry C, 2014, 118, 15242-15250.	3.1	33
39	Surface composition of magnetron sputtered Pt-Co thin film catalyst for proton exchange membrane fuel cells. Applied Surface Science, 2016, 365, 245-251.	6.1	33
40	Methane dry reforming on supported cobalt nanoparticles promoted by boron. Journal of Catalysis, 2020, 392, 126-134.	6.2	32
41	Roughening of Copper (100) at Elevated CO Pressure: Cu Adatom and Cluster Formation Enable CO Dissociation. Journal of Physical Chemistry C, 2019, 123, 8112-8121.	3.1	30
42	Versatile Optimization of Chemical Ordering in Bimetallic Nanoparticles. Journal of Physical Chemistry C, 2017, 121, 10803-10808.	3.1	29
43	Catalysis from First Principles: Towards Accounting for the Effects of Nanostructuring. Topics in Catalysis, 2013, 56, 867-873.	2.8	28
44	Theoretical study of carbon species on Pd(111): competition between migration of C atoms to the subsurface interlayer and formation of Cn clusters on the surface. Physical Chemistry Chemical Physics, 2009, 11, 10955.	2.8	27
45	Energetic Stability of Absorbed H in Pd and Pt Nanoparticles in a More Realistic Environment. Journal of Physical Chemistry C, 2015, 119, 5180-5186.	3.1	25
46	Revealing chemical ordering in Ptâ€"Co nanoparticles using electronic structure calculations and X-ray photoelectron spectroscopy. Physical Chemistry Chemical Physics, 2015, 17, 28298-28310.	2.8	24
47	Electrochemical Conversion of CO₂ to 2-Bromoethanol in a Membraneless Cell. ACS Energy Letters, 2019, 4, 600-605.	17.4	21
48	Revamping SiO₂ Spheres by Coreâ€"Shell Porosity Endowment to Construct a Mazelike Nanoreactor for Enhanced Catalysis in CO₂ Hydrogenation to Methanol. Advanced Functional Materials, 2021, 31, 2102896.	14.9	21
49	Reduced ceria nanofilms from structure prediction. Nanoscale, 2015, 7, 4361-4366.	5.6	20
50	Synthesis of Mesoporous Copper Aluminosilicate Hollow Spheres for Oxidation Reactions. ACS Applied Materials & Interfaces, 2020, 12, 23060-23075.	8.0	17
51	[Ag₉(1,2-BDT)₆]^{3â€"}: How Square-Pyramidal Building Blocks Self-Assemble into the Smallest Silver Nanocluster. Inorganic Chemistry, 2021, 60, 4306-4312.	4.0	16
52	Bonding and vibrations of CHxO and CHx species (x=1â€"3) on a palladium nanoparticle representing model catalysts. Chemical Physics Letters, 2011, 506, 92-97.	2.6	15
53	Stereoisomerization during Molecular Packing. Advanced Materials, 2021, 33, e2100986.	21.0	13
54	Quantifying interactions on interfaces between metal particles and oxide supports in catalytic nanomaterials. NPG Asia Materials, 2022, 14, .	7.9	12

#	ARTICLE	IF	CITATIONS
55	Atomic Ordering and Sn Segregation in Ptâ€“Sn Nanoalloys Supported on CeO2 Thin Films. Topics in Catalysis, 2017, 60, 522-532.	2.8	11
56	Steering the formation of supported Ptâ€“Sn nanoalloys by reactive metalâ€“oxide interaction. RSC Advances, 2016, 6, 85688-85697.	3.6	5
57	Approaching complexity of alkyl hydrogenation on Pd via density-functional modelling. Physical Chemistry Chemical Physics, 2017, 19, 21514-21521.	2.8	3
58	Revamping SiO₂ Spheres by Coreâ€“Shell Porosity Endowment to Construct a Mazelike Nanoreactor for Enhanced Catalysis in CO₂ Hydrogenation to Methanol (Adv. Funct.) Tj ETQq0 0 0 rgBT /Overlock 10 Tf 50	14.9	3
59	From Static to Reacting Systems on Transition-Metal Surfaces. , 2013, , 475-503.		2