Sergey M Kozlov

List of Publications by Citations

59 papers	2,871 citations	30 h-index	53 g-index
61 ext. papers	3,507 ext. citations	10.1 avg, IF	5.2 L-index

#	Paper	IF	Citations
59	Counting electrons on supported nanoparticles. *Nature Materials*, **2016**, 15, 284-8	27	325
58	Bulk Properties of Transition Metals: A Challenge for the Design of Universal Density Functionals. *Journal of Chemical Theory and Computation*, **2014**, 10, 3832-9	6.4	187
57	Establishing the Accuracy of Broadly Used Density Functionals in Describing Bulk Properties of Transition Metals. *Journal of Chemical Theory and Computation*, **2013**, 9, 1631-40	6.4	153
56	High-valence metals improve oxygen evolution reaction performance by modulating 3d metal oxidation cycle energetics. *Nature Catalysis*, **2020**, 3, 985-992	36.5	149
55	Graphene on Ni(111): Coexistence of Different Surface Structures. *Journal of Physical Chemistry Letters*, **2011**, 2, 759-764	6.4	139
54	Bonding Mechanisms of Graphene on Metal Surfaces. *Journal of Physical Chemistry C*, **2012**, 116, 7360-7368	4.8	121
53	Water Chemistry on Model Ceria and Pt/Ceria Catalysts. *Journal of Physical Chemistry C*, **2012**, 116, 12103-12113	4.8	93
52	The role of metal/oxide interfaces for long-range metal particle activation during CO oxidation. *Nature Materials*, **2018**, 17, 519-522	27	89
51	Quantum-Dot-Derived Catalysts for CO2 Reduction Reaction. *Joule*, **2019**, 3, 1703-1718	27.8	78
50	Solution processable metal-organic frameworks for mixed matrix membranes using porous liquids. *Nature Materials*, **2020**, 19, 1346-1353	27	78
49	Bandgap engineering of graphene by physisorbed adsorbates. *Advanced Materials*, **2011**, 23, 2638-43	24	75
48	Growth and electronic structure of nitrogen-doped graphene on Ni(111). *Physical Review B*, **2012**, 86,	3.3	73
47	Doping-Induced Anisotropic Self-Assembly of Silver Icosahedra in [PtAgCl(PPh)] Nanoclusters. *Journal of the American Chemical Society*, **2017**, 139, 1053-1056	16.4	67
46	How absorbed hydrogen affects the catalytic activity of transition metals. *Angewandte Chemie - International Edition*, **2014**, 53, 13371-5	16.4	63
45	On the interaction of polycyclic aromatic compounds with graphene. *Carbon*, **2012**, 50, 2482-2492	10.4	61
44	In-operando elucidation of bimetallic CoNi nanoparticles during high-temperature CH4/CO2 reaction. *Applied Catalysis B: Environmental*, **2017**, 213, 177-189	21.8	60
43	Tailoring the Crystal Structure of Nanoclusters Unveiled High Photoluminescence via Ion Pairing. *Chemistry of Materials*, **2018**, 30, 2719-2725	9.6	60

42	How to determine accurate chemical ordering in several nanometer large bimetallic crystallites from electronic structure calculations. *Chemical Science*, **2015**, 6, 3868-3880	9.4	58
41	Formation of one-dimensional electronic states along the step edges of CeO(111). *ACS Nano*, **2012**, 6, 1126-33	16.7	55
40	Turning a Methanation Co Catalyst into an In-Co Methanol Producer. *ACS Catalysis*, **2019**, 9, 6910-6918	13.1	54
39	Theoretical assessment of graphene-metal contacts. *Journal of Chemical Physics*, **2013**, 138, 244701	3.9	53
38	Direct versus ligand-exchange synthesis of [PtAg(BDT)(TPP)] nanoclusters: effect of a single-atom dopant on the optoelectronic and chemical properties. *Nanoscale*, **2017**, 9, 9529-9536	7.7	47
37	Constructing Bridges between Computational Tools in Heterogeneous and Homogeneous Catalysis. *ACS Catalysis*, **2018**, 8, 5637-5656	13.1	42
36	Stabilization of Small Platinum Nanoparticles on Pt-CeO2 Thin Film Electrocatalysts During Methanol Oxidation. *Journal of Physical Chemistry C*, **2016**, 120, 19723-19736	3.8	42
35	Surface composition changes of CuNi-ZrO2 during methane decomposition: An operando NAP-XPS and density functional study. *Catalysis Today*, **2017**, 283, 134-143	5.3	40
34	Tandem Conversion of CO2 to Valuable Hydrocarbons in Highly Concentrated Potassium Iron Catalysts. *ChemCatChem*, **2019**, 11, 2879-2886	5.2	37
33	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	3.8	37
32	Absolute Surface Step Energies: Accurate Theoretical Methods Applied to Ceria Nanoislands. *Journal of Physical Chemistry Letters*, **2012**, 3, 1956-1961	6.4	35
31	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	3.9	35
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	7.3	33
29	Insights from methane decomposition on nanostructured palladium. *Journal of Catalysis*, **2016**, 337, 111-121	7.3	29
28	O vacancies on steps on the CeO2(111) surface. *Physical Chemistry Chemical Physics*, **2014**, 16, 7823-9	3.6	28
27	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	3.8	28
26	Surface composition of magnetron sputtered Pt-Co thin film catalyst for proton exchange membrane fuel cells. *Applied Surface Science*, **2016**, 365, 245-251	6.7	27
25	Efficient electrochemical transformation of CO to C/C chemicals on benzimidazole-functionalized copper surfaces. *Chemical Communications*, **2018**, 54, 11324-11327	5.8	27

24	Versatile Optimization of Chemical Ordering in Bimetallic Nanoparticles. *Journal of Physical Chemistry C*, **2017**, 121, 10803-10808	3.8	26
23	Oxygen vacancies in self-assemblies of ceria nanoparticles. *Journal of Materials Chemistry A*, **2014**, 2, 18329-18338	13	26
22	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, 10955-63	3.6	25
21	Role of Oxidized Mo Species on the Active Surface of NiMo Electrocatalysts for Hydrogen Evolution under Alkaline Conditions. *ACS Catalysis*, **2020**, 10, 12858-12866	13.1	24
20	Catalysis from First Principles: Towards Accounting for the Effects of Nanostructuring. *Topics in Catalysis*, **2013**, 56, 867-873	2.3	22
19	Energetic Stability of Absorbed H in Pd and Pt Nanoparticles in a More Realistic Environment. *Journal of Physical Chemistry C*, **2015**, 119, 5180-5186	3.8	21
18	Revealing chemical ordering in Pt-Co nanoparticles using electronic structure calculations and X-ray photoelectron spectroscopy. *Physical Chemistry Chemical Physics*, **2015**, 17, 28298-310	3.6	19
17	Electronic-structure-based material descriptors: (in)dependence on self-interaction and Hartree-Fock exchange. *Chemical Communications*, **2015**, 51, 5602-5	5.8	17
16	Reduced ceria nanofilms from structure prediction. *Nanoscale*, **2015**, 7, 4361-6	7.7	15
15	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	3.8	15
14	Bonding and vibrations of CHxO and CHx species (x=1–3) on a palladium nanoparticle representing model catalysts. *Chemical Physics Letters*, **2011**, 506, 92-97	2.5	14
13	Methane dry reforming on supported cobalt nanoparticles promoted by boron. *Journal of Catalysis*, **2020**, 392, 126-134	7.3	11
12	Atomic Ordering and Sn Segregation in Pt–Sn Nanoalloys Supported on CeO2 Thin Films. *Topics in Catalysis*, **2017**, 60, 522-532	2.3	10
11	How Absorbed Hydrogen Affects the Catalytic Activity of Transition Metals. *Angewandte Chemie*, **2014**, 126, 13589-13593	3.6	9
10	Synthesis of Mesoporous Copper Aluminosilicate Hollow Spheres for Oxidation Reactions. *ACS Applied Materials & Interfaces*, **2020**, 12, 23060-23075	9.5	7
9	Atomic Pd-promoted ZnZrO solid solution catalyst for CO2 hydrogenation to methanol. *Applied Catalysis B: Environmental*, **2022**, 304, 120994	21.8	7
8	Electrochemical Conversion of CO2 to 2-Bromoethanol in a Membraneless Cell. *ACS Energy Letters*, **2019**, 4, 600-605	20.1	6
7	Steering the formation of supported Pt–Sn nanoalloys by reactive metal–oxide interaction. *RSC Advances*, **2016**, 6, 85688-85697	3.7	5

6	[Ag(1,2-BDT)]: How Square-Pyramidal Building Blocks Self-Assemble into the Smallest Silver Nanocluster. *Inorganic Chemistry*, **2021**, 60, 4306-4312	5.1	3
5	Stereoisomerization during Molecular Packing. *Advanced Materials*, **2021**, 33, e2100986	24	3
4	Approaching complexity of alkyl hydrogenation on Pd via density-functional modelling. *Physical Chemistry Chemical Physics*, **2017**, 19, 21514-21521	3.6	2
3	From Static to Reacting Systems on Transition-Metal Surfaces **2013**, 475-503		2
2	Revamping SiO2 Spheres by Core–Shell Porosity Endowment to Construct a Mazelike Nanoreactor for Enhanced Catalysis in CO2 Hydrogenation to Methanol. *Advanced Functional Materials*, **2021**, 31, 2102896	15.6	2
1	Revamping SiO2 Spheres by Core–Shell Porosity Endowment to Construct a Mazelike Nanoreactor for Enhanced Catalysis in CO2 Hydrogenation to Methanol (Adv. Funct. Mater. 47/2021). *Advanced Functional Materials*, **2021**, 31, 2170345	15.6	1