Ilya V Yudanov

List of Publications by Year
in descending order

43	2,515	186265	254184
papers	citations	28 h-index	43 g-index

45	45	45	2084
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	Systematic Density Functional Study of the Adsorption of Transition Metal Atoms on the MgO(001) Surface. Journal of Physical Chemistry B, 1997, 101, 2786-2792.	2.6	272
2	CO Adsorption on Pd Nanoparticles:Â Density Functional and Vibrational Spectroscopy Studies. Journal of Physical Chemistry B, 2003, 107, 255-264.	2.6	262
3	Adsorption of transition metal atoms on oxygen vacancies and regular sites of the MgO(001) surface. Surface Science, 1999, 426, 123-139.	1.9	165
4	Size Dependence of the Adsorption Energy of CO on Metal Nanoparticles: A DFT Search for the Minimum Value. Nano Letters, 2012, 12, 2134-2139.	9.1	155
5	Metal nanoparticles as models of single crystal surfaces and supported catalysts: Density functional study of size effects for CO/Pd(111). Journal of Chemical Physics, 2002, 117, 9887-9896.	3.0	144
6	Trigonal-Bipyramidal Lewis Base Adducts of Methyltrioxorhenium(VII) and Their Bisperoxo Congeners: Characterization, Application in Catalytic Epoxidation, and Density Functional Mechanistic Study. Chemistry - A European Journal, 1999, 5, 3603-3615.	3.3	122
7	Density functional study of Pd nanoparticles with subsurface impurities of light element atoms. Physical Chemistry Chemical Physics, 2004, 6, 116-123.	2.8	105
8	Adsorption of Pd atoms and Pd4 clusters on the MgO(001) surface: a density functional study. Chemical Physics Letters, 1997, 275, 245-252.	2.6	88
9	Olefin Epoxidation by Peroxo Complexes of Cr, Mo, and W. A Comparative Density Functional Study. Journal of Organic Chemistry, 2000, 65, 2996-3004.	3.2	87
10	Size-Dependence of Adsorption Properties of Metal Nanoparticles: A Density Functional Study on Palladium Nanoclusters. Journal of Physical Chemistry C, 2008, 112, 20269-20275.	3.1	86
11	How the Câ^'O Bond Breaks during Methanol Decomposition on Nanocrystallites of Palladium Catalysts. Journal of the American Chemical Society, 2008, 130, 9342-9352.	13.7	77
12	Particle-size dependent heats of adsorption of CO on supported Pd nanoparticles as measured with a single-crystal microcalorimeter. Physical Review B, 2010, 81, .	3.2	77
13	Olefin Epoxidation by Molybdenum and Rhenium Peroxo and Hydroperoxo Compounds:â€‰ A Density Functional Study of Energetics and Mechanisms. Inorganic Chemistry, 2001, 40, 3755-3765.	4.0	73
14	Density functional cluster description of ionic materials: Improved boundary conditions for MgO clusters with the help of cation model potentials. International Journal of Quantum Chemistry, 1997, 65, 975-986.	2.0	69
15	Activity of Peroxo and Hydroperoxo Complexes of TiIV in Olefin Epoxidation: A Density Functional Model Study of Energetics and Mechanism. European Journal of Inorganic Chemistry, 1999, 1999, 2135-2145.	2.0	58
16	Stabilization of Au at edges of bimetallic PdAu nanocrystallites. Physical Chemistry Chemical Physics, 2010, 12, 5094.	2.8	57
17	Olefin epoxidation by mono and bisperoxo complexes of Mo(VI): a density functional model study. Journal of Molecular Catalysis A, 2000, 158, 189-197.	4.8	51
18	Mechanism of Selective Hydrogenation of Î±,Î²-Unsaturated Aldehydes on Silver Catalysts: A Density Functional Study. Journal of Physical Chemistry C, 2009, 113, 13231-13240.	3.1	47

#	Article	IF	Citations
19	Hydrogen Activation on Silver:â€‰ A Computational Study on Surface and Subsurface Oxygen Species. Journal of Physical Chemistry C, 2008, 112, 1628-1635.	3.1	44
20	A computational study of H2dissociation on silver surfaces: The effect of oxygen in the added row structure of Ag(110). Physical Chemistry Chemical Physics, 2007, 9, 1247-1254.	2.8	43
21	Molecular models of catalytically active sites in zeolites. Quantum chemical approach. Catalysis Today, 1999, 51, 397-410.	4.4	40
22	Pd Segregation on the Surface of Bimetallic PdAu Nanoparticles Induced by Low Coverage of Adsorbed CO. Journal of Physical Chemistry C, 2019, 123, 8037-8046.	3.1	40
23	DFT Studies of Palladium Model Catalysts: Structure and Size Effects. Journal of Cluster Science, 2011, 22, 433-448.	3.3	39
24	Size-Dependence of the Adsorption Energy of CO on Pt Nanoparticles: Tracing Two Intersecting Trends by DFT Calculations. Journal of Physical Chemistry C, 2017, 121, 17371-17377.	3.1	39
25	Cluster Quantum Chemical Study of the Interaction of Dimethyl Methylphosphonate with Magnesium Oxide. The Journal of Physical Chemistry, 1994, 98, 10032-10035.	2.9	38
26	Adsorption of carbon on Pd clusters of nanometer size: A first-principles theoretical study. Journal of Chemical Physics, 2005, 122, 174705.	3.0	33
27	Adsorption of Cu4, Ag4 and Au4 particles on the regular MgO(001) surface: A density functional study using embedded cluster models. Chemical Physics Letters, 2006, 417, 515-520.	2.6	33
28	Mechanism of olefin epoxidation with transition metal peroxo complexes: DFT study. Journal of Structural Chemistry, 2007, 48, S111-S124.	1.0	32
29	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
30	Câ€“O bond scission of methoxide on Pd nanoparticles: A density functional study. Physical Chemistry Chemical Physics, 2006, 8, 2396-2401.	2.8	24
31	Density functional study of SO2 adsorption in HY zeolites. Computational and Theoretical Chemistry, 1999, 466, 235-244.	1.5	11
32	Molecular models of active sites of C1 and C2 hydrocarbon activation. Catalysis Today, 1995, 24, 383-387.	4.4	10
33	Chelate complex Ni(S2C2H2)2 as a molecular model of the hydrodesulfurization active center. Reaction Kinetics and Catalysis Letters, 1997, 61, 117-122.	0.6	10
34	Mechanism of Olefin Epoxidation by Transition Metal Peroxo Compounds. Catalysis By Metal Complexes, 2002, , 289-324.	0.6	10
35	Scalable properties of metal clusters: A comparative DFT study of ionic-core treatments. Chemical Physics Letters, 2013, 578, 92-96.	2.6	8
36	Pd Single-Atom Sites on the Surface of PdAu Nanoparticles: A DFT-Based Topological Search for Suitable Compositions. Nanomaterials, 2021, 11, 122.	4.1	8

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37	Ab initio quantum chemical calculation of the electronic structure of the chelate complex Ni(S2C2H2)2. Journal of Structural Chemistry, 1996, 37, 201-205.	1.0	7
38	Simulation of heterogeneous catalysts and catalytic processes using the density functional method. Kinetics and Catalysis, 2010, 51, 832-842.	1.0	4
39	Quantum chemical treatment of active sites in zeolites. Reaction Kinetics and Catalysis Letters, 1996, 57, 263-274.	0.6	3
40	Theoretical Study of the Methanol Dehydrogenation on Platinum Nanocluster. Journal of Siberian Federal University: Chemistry, 2016, 9, 430-442.	0.7	3
41	Size and structure effects on platinum nanocatalysts: theoretical insights from methanol dehydrogenation. Nanoscale, 2022, 14, 4145-4155.	5.6	3
42	Copper hydroxide catalysts for selective oxidation: Quantum chemical study of active sites. Reaction Kinetics and Catalysis Letters, 2004, 82, 347-354.	0.6	2
43	Trigonal-Bipyramidal Lewis Base Adducts of Methyltrioxorhenium(VII) and Their Bisperoxo Congeners: Characterization, Application in Catalytic Epoxidation, and Density Functional Mechanistic Study. Chemistry - A European Journal, 1999, 5, 3603-3615.	3.3	1