# 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 | Size and structure effects on platinum nanocatalysts: theoretical insights from methanol dehydrogenation. Nanoscale, 2022, 14, 4145-4155. | 5.6 | 3 |
| 2 | 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 |
| 3 | 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 |
| 4 | 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 |
| 5 | Theoretical Study of the Methanol Dehydrogenation on Platinum Nanocluster. Journal of Siberian Federal University: Chemistry, 2016, 9, 430-442. | 0.7 | 3 |
| 6 | Scalable properties of metal clusters: A comparative DFT study of ionic-core treatments. Chemical Physics Letters, 2013, 578, 92-96. | 2.6 | 8 |
| 7 | 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 |
| 8 | DFT Studies of Palladium Model Catalysts: Structure and Size Effects. Journal of Cluster Science, 2011, 22, 433-448. | 3.3 | 39 |
| 9 | Simulation of heterogeneous catalysts and catalytic processes using the density functional method. Kinetics and Catalysis, 2010, 51, 832-842. | 1.0 | 4 |
| 10 | Stabilization of Au at edges of bimetallic PdAu nanocrystallites. Physical Chemistry Chemical Physics, 2010, 12, 5094. | 2.8 | 57 |
| 11 | 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 |
| 12 | 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 |
| 13 | 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 |
| 14 | 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 |
| 15 | 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 |
| 16 | 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 |
| 17 | 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 |
| 18 | Mechanism of olefin epoxidation with transition metal peroxo complexes: DFT study. Journal of Structural Chemistry, 2007, 48, S111-S124. | 1.0 | 32 |

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|---|---|---|---|
| 19 | Câ€“O bond scission of methoxide on Pd nanoparticles: A density functional study. Physical Chemistry Chemical Physics, 2006, 8, 2396-2401. | 2.8 | 24 |
| 20 | 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 |
| 21 | Adsorption of carbon on Pd clusters of nanometer size: A first-principles theoretical study. Journal of Chemical Physics, 2005, 122, 174705. | 3.0 | 33 |
| 22 | Copper hydroxide catalysts for selective oxidation: Quantum chemical study of active sites. Reaction Kinetics and Catalysis Letters, 2004, 82, 347-354. | 0.6 | 2 |
| 23 | Density functional study of Pd nanoparticles with subsurface impurities of light element atoms. Physical Chemistry Chemical Physics, 2004, 6, 116-123. | 2.8 | 105 |
| 24 | CO Adsorption on Pd Nanoparticles:Â Density Functional and Vibrational Spectroscopy Studies. Journal of Physical Chemistry B, 2003, 107, 255-264. | 2.6 | 262 |
| 25 | 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 |
| 26 | Mechanism of Olefin Epoxidation by Transition Metal Peroxo Compounds. Catalysis By Metal Complexes, 2002, , 289-324. | 0.6 | 10 |
| 27 | 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 |
| 28 | 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 |
| 29 | 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 |
| 30 | Molecular models of catalytically active sites in zeolites. Quantum chemical approach. Catalysis Today, 1999, 51, 397-410. | 4.4 | 40 |
| 31 | Density functional study of SO2 adsorption in HY zeolites. Computational and Theoretical Chemistry, 1999, 466, 235-244. | 1.5 | 11 |
| 32 | 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 |
| 33 | 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 |
| 34 | 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 |
| 35 | 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 |
| 36 | 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 |

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|---|---|---|---|
| 37 | 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 |
| 38 | 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 |
| 39 | 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 |
| 40 | Quantum chemical treatment of active sites in zeolites. Reaction Kinetics and Catalysis Letters, 1996, 57, 263-274. | 0.6 | 3 |
| 41 | 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 |
| 42 | Molecular models of active sites of C1 and C2 hydrocarbon activation. Catalysis Today, 1995, 24, 383-387. | 4.4 | 10 |
| 43 | 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 |