Lyudmila V Moskaleva

List of Publications by Year
in descending order

71	2,472	230014 27	232693 48
papers	citations	h-index	g-index

76	76	76	3105
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	Ultrathin Metal Silicate Hydroxide Nanosheets with Moderate Metalâ€“Oxygen Covalency Enables Efficient Oxygen Evolution. Energy and Environmental Materials, 2022, 5, 231-237.	7.3	28
2	First-Principles Study of the Electronic Properties and Thermal Expansivity of a Hybrid 2D Carbon and Boron Nitride Material. Journal of Carbon Research, 2021, 7, 5.	1.4	1
3	Atomically dispersed nonmagnetic electron traps improve oxygen reduction activity of perovskite oxides. Energy and Environmental Science, 2021, 14, 1016-1028.	15.6	130
4	Transient Auâ€“CO Complexes Promote the Activity of an Inverse Ceria/Gold Catalyst: An Insight from Ab Initio Molecular Dynamics. Journal of Physical Chemistry C, 2021, 125, 26406-26417.	1.5	2
5	Combined Relativistic Ab Initio Multireference and Experimental Study of the Electronic Structure of Terbium Luminescent Compound. Journal of Physical Chemistry A, 2020, 124, 82-89.	1.1	5
6	Tuning the electronic structure and thermodynamic properties of hybrid graphene-hexagonal boron nitride monolayer. FlatChem, 2020, 24, 100194.	2.8	6
7	Assessment of PBE+U and HSE06 methods and determination of optimal parameter U for the structural and energetic properties of rare earth oxides. Journal of Chemical Physics, 2020, 153, 164710.	1.2	13
8	Tuning Oxygen Vacancies of Oxides to Promote Electrocatalytic Reduction of Carbon Dioxide. ACS Energy Letters, 2020, 5, 552-558.	8.8	54
9	What Changes on the Inverse Catalyst? Insights from CO Oxidation on Au-Supported Ceria Nanoparticles Using Ab Initio Molecular Dynamics. ACS Catalysis, 2020, 10, 3164-3174.	5.5	11
10	Formation of One-Dimensional Coordination Chains for High-Performance Anode Materials of Lithium-Ion Batteries via a Bottom-Up Approach. ACS Applied Materials & Interfaces, 2019, 11, 25863-25869.	4.0	19
11	Understanding Oxygen Activation on Nanoporous Gold. ACS Catalysis, 2019, 9, 5204-5216.	5.5	26
12	Sisyphus effects in hydrogen electrochemistry on metal silicides enabled by silicene subunit edge. Science Bulletin, 2019, 64, 617-624.	4.3	65
13	CO Adsorption on Au(332): Combined Infrared Spectroscopy and Density Functional Theory Study. Journal of Physical Chemistry C, 2019, 123, 8187-8197.	1.5	7
14	CO Oxidation over Unsupported Group 11 Metal Catalysts: New Mechanistic Insight from First-Principles. Journal of Physical Chemistry C, 2019, 123, 7818-7830.	1.5	8
15	MoB/gâ€₃N₄ Interface Materials as a Schottky Catalyst to Boost Hydrogen Evolution. Angewandte Chemie, 2018, 130, 505-509.	1.6	71
16	MoB/gâ€₃N₄ Interface Materials as a Schottky Catalyst to Boost Hydrogen Evolution. Angewandte Chemie - International Edition, 2018, 57, 496-500.	7.2	308
17	Oxygen-Driven Surface Evolution of Nanoporous Gold: Insights from Ab Initio Molecular Dynamics and Auger Electron Spectroscopy. Journal of Physical Chemistry C, 2018, 122, 5349-5357.	1.5	25
18	Tracking down the origin of peculiar vibrational spectra of aromatic self-assembled thiolate monolayers. Physical Chemistry Chemical Physics, 2018, 20, 29918-29930.	1.3	6

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19	Aerobic Alcohol Oxidation on Nanoporous Gold: Toward a Mechanistic Understanding of the Reactivity. , 2018, , 20-30.		2
20	Methanol oxidation on the Au(3â€¯1â€¯0) surface: A theoretical study. Journal of Catalysis, 2018, 364, 216-227.	3.1	17
21	How silver segregation stabilizes 1D surface gold oxide: a cluster expansion study combined with ab initio MD simulations. Physical Chemistry Chemical Physics, 2017, 19, 14845-14853.	1.3	23
22	Theoretical mechanistic insights into propylene epoxidation on Au-based catalysts: Surface O versus OOH as oxidizing agents. Catalysis Today, 2016, 278, 45-55.	2.2	21
23	Transformations of Organic Molecules over Metal Surfaces: Insights from Computational Catalysis. Chemical Record, 2016, 16, 2388-2404.	2.9	14
24	Chemisorbed Oxygen on the Au(321) Surface Alloyed with Silver: A First-Principles Investigation. Journal of Physical Chemistry C, 2015, 119, 9215-9226.	1.5	41
25	Ab Initio Chemical Kinetics for H + NCN: Prediction of NCN Heat of Formation and Reaction Product Branching via Doublet and Quartet Surfaces. Journal of Physical Chemistry A, 2013, 117, 5775-5784.	1.1	19
26	Formation of n-hexane from methylcyclopentane via a metallacyclobutane intermediate at step sites of Pt surfaces: Mechanism from first-principles calculations. Journal of Catalysis, 2013, 299, 146-149.	3.1	10
27	Ring-Opening Reactions of Methylcyclopentane over Metal Catalysts, M = Pt, Rh, Ir, and Pd: A Mechanistic Study from First-Principles Calculations. ACS Catalysis, 2013, 3, 196-205.	5.5	33
28	From Static to Reacting Systems on Transition-Metal Surfaces. , 2013, , 475-503.		2
29	CO oxidation by co-adsorbed atomic O on the Au(321) surface with Ag impurities: A mechanistic study from first-principles calculations. Chemical Physics Letters, 2012, 525-526, 87-91.	1.2	26
30	Tuning the selectivity for ring-opening reactions of methylcyclopentane over Pt catalysts: A mechanistic study from first-principles calculations. Journal of Catalysis, 2012, 285, 124-133.	3.1	38
31	Ethylene conversion to ethylidyne on Pd(111) and Pt(111): A first-principles-based kinetic Monte Carlo study. Journal of Catalysis, 2012, 285, 187-195.	3.1	66
32	Silver residues as a possible key to a remarkable oxidative catalytic activity of nanoporous gold. Physical Chemistry Chemical Physics, 2011, 13, 4529.	1.3	121
33	Angular distributions of electrons emitted from free and deposited Na₈ clusters. Physica Status Solidi (B): Basic Research, 2010, 247, 1122-1131.	0.7	1
34	Comparative density functional study of the complexes [UO2(CO3)3]4â^' and [(UO2)3(CO3)6]6â^' in aqueous solution. Dalton Transactions, 2010, 39, 5705.	1.6	15
35	Ethylidyne Formation from Ethylene over Pt(111): A Mechanistic Study from First-Principle Calculations. Journal of Physical Chemistry C, 2010, 114, 12190-12201.	1.5	77
36	Modeling of the deposition of Na Clusters on MgO(001). Physical Review B, 2009, 80, .	1.1	6

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37	Ethylene Conversion to Ethylidyne over Pd(111): Revisiting the Mechanism with First-Principles Calculations. Journal of Physical Chemistry C, 2009, 113, 2512-2520.	1.5	56
38	Ethylidyne Formation from Ethylene over Pd(111): Alternative Routes from a Density Functional Study. Journal of Physical Chemistry C, 2009, 113, 15373-15379.	1.5	29
39	Characterization of optical spectra of interacting systems: Application to oxideâ€supported metal clusters. International Journal of Quantum Chemistry, 2008, 108, 2978-2990.	1.0	3
40	DYNAMICS OF METAL CLUSTERS: FREE, EMBEDDED AND DEPOSITED. , 2008, , 273-282.		0
41	Microscopic models of PdZn alloy catalysts: structure and reactivity in methanol decomposition. Physical Chemistry Chemical Physics, 2007, 9, 3470-3482.	1.3	96
42	Optical Spectra of Cu, Ag, and Au Monomers and Dimers at Regular Sites and Oxygen Vacancies of the MgO(001) Surface. A Systematic Time-Dependent Density Functional Study Using Embedded Cluster Modelsâ€. Journal of Physical Chemistry A, 2007, 111, 6870-6880.	1.1	9
43	Density Functional Embedded Cluster Study of Cu4, Ag4and Au4Species Interacting with Oxygen Vacancies on the MgO(001) Surface. Chemistry - A European Journal, 2007, 13, 277-286.	1.7	22
44	Structure and optical properties of Na clusters deposited on MgO(001). European Physical Journal D, 2007, 45, 507-514.	0.6	14
45	The heat of formation of gaseous PuO22+from relativistic density functional calculations. Physical Chemistry Chemical Physics, 2006, 8, 3767-3773.	1.3	13
46	Modeling Adsorption of the Uranyl Dication on the Hydroxylated Î±-Al2O3(0001) Surface in an Aqueous Medium. Density Functional Study. Langmuir, 2006, 22, 2141-2145.	1.6	49
47	Systematic DFT Study of Gas Phase and Solvated Uranyl and Neptunyl Complexes [AnO2X4]n(An = U, Np;) Tj ETQq1 1 0.784314 rgBT	1.9	41
48	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.	1.2	33
49	Adsorption of dimers and trimers of Cu, Ag, and Au on regular sites and oxygen vacancies of the MgO(001) surface: a density functional study using embedded cluster models. Applied Physics A: Materials Science and Processing, 2006, 82, 181-189.	1.1	52
50	The Heat of Formation of the Uranyl Dication: Theoretical Evaluation Based on Relativistic Density Functional Calculations. Chemistry - A European Journal, 2006, 12, 629-634.	1.7	17
51	Surface Composition of Materials Used as Catalysts for Methanol Steam Reforming: A Theoretical Study. ChemPhysChem, 2006, 7, 1802-1812.	1.0	26
52	Lewis base interaction with gallium hydrides: a computational study. Inorganica Chimica Acta, 2005, 358, 4163-4171.	1.2	0
53	Electronic structure and screening dynamics of ethene on single-domain Si(001) from resonant inelastic x-ray scattering. Physical Review B, 2004, 69, .	1.1	6
54	Quantum chemistry with the Douglas-Kroll-Hess approach to relativistic density functional theory: Efficient methods for molecules and materials. Theoretical and Computational Chemistry, 2004, 14, 656-722.	0.2	32

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55	Quantum chemical/vRRKM study on the thermal decomposition of cyclopentadiene. International Journal of Chemical Kinetics, 2004, 36, 139-151.	1.0	21
56	Role of Solvation in the Reduction of the Uranyl Dication by Water: A Density Functional Study. ChemInform, 2004, 35, no.	0.1	0
57	Elastic polarizable environment cluster embedding approach for water adsorption on the Î±-Al2O3(0001) surface. A density functional study. Physical Chemistry Chemical Physics, 2004, 6, 4505-4513.	1.3	16
58	Role of Solvation in the Reduction of the Uranyl Dication by Water:Â A Density Functional Study. Inorganic Chemistry, 2004, 43, 4080-4090.	1.9	65
59	Computational Study of the HCCO + NO Reaction:Â ab Initio MO/vRRKM Calculations of the Total Rate Constant and Product Branching Ratios. Journal of Physical Chemistry A, 2003, 107, 1066-1076.	1.1	32
60	Computational study of the kinetics and mechanisms for the reaction of H atoms with c-C5H6. Proceedings of the Combustion Institute, 2002, 29, 1319-1327.	2.4	14
61	Computational Study on the Energetics of NCN Isomers and the Kinetics of the C + N2â‡„ N + CN Reaction. Journal of Physical Chemistry A, 2001, 105, 4156-4163.	1.1	30
62	The CH + N2 Association Reaction at Low Temperatures: Ab Initio MO/VRRKM-Theory Analysis of Temperature and Pressure Effects. Zeitschrift Fur Physikalische Chemie, 2001, 215, .	1.4	4
63	The spin-conserved reaction CH+N2â†'H+NCN: A major pathway to prompt no studied by quantum/statistical theory calculations and kinetic modeling of rate constant. Proceedings of the Combustion Institute, 2000, 28, 2393-2401.	2.4	145
64	The CH+N2 reaction over the ground electronic doublet potential energy surface: a detailed transition state search. Chemical Physics Letters, 2000, 331, 269-277.	1.2	67
65	Ab initio MO calculations for the reactions of NH2 with H2, H2O, NH3 and CH4: prediction of absolute rate constants and kinetic isotope effects. Computational and Theoretical Chemistry, 1999, 461-462, 223-238.	1.5	16
66	Unimolecular isomerization/decomposition of ortho-benzyne: ab initio MO/statistical theory study. Physical Chemistry Chemical Physics, 1999, 1, 3967-3972.	1.3	57
67	Theoretical Study of the NH2+ C2H2Reaction. Journal of Physical Chemistry A, 1998, 102, 4687-4693.	1.1	16
68	Thermal decomposition of formic acid in the gas phase: bimolecular and H2O catalysed reactions. Molecular Physics, 1997, 92, 581-586.	0.8	23
69	Ab Initio MO Study of the Unimolecular Decomposition of the Phenyl Radical. Journal of Physical Chemistry A, 1997, 101, 6790-6797.	1.1	77
70	The CH3+C5H5 reaction: A potential source of benene at high temperatures. Proceedings of the Combustion Institute, 1996, 26, 521-526.	0.3	71
71	Origins of the High Reactivity of Au Nanostructures Deduced from the Structure and Properties of Model Surfaces. , 0, , .		1