Alexei M Shor

List of Publications by Year
in descending order

31	464	759233 12	713466 21
papers	citations	h-index	g-index

33	33	33	606
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	Adsorption and Oxidation of CO on Ceria Nanoparticles Exposing Single-Atom Pd and Ag: A DFT Modelling. Materials, 2021, 14, 6888.	2.9	2
3	Manganeseâ€“goldâ€“manganese complex with vinylidene and acetylide units. Dalton Transactions, 2020, 49, 17527-17531.	3.3	2
4	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.	11.2	11
5	Hydration Structure and Hydrolysis of U(IV) and Np(IV) Ions: A Comparative Density Functional Study Using a Modified Continuum Solvation Approach. Journal of Physical Chemistry A, 2020, 124, 3805-3814.	2.5	3
6	Silver atom, trimer and tetramer species supported on a ceria nanoparticle: A density functional study. Surface Science, 2019, 681, 38-46.	1.9	8
7	Theoretical study of O2 interaction with subnanometer-sized Ag clusters supported on defective SiO2 surface. Computational and Theoretical Chemistry, 2018, 1144, 56-65.	2.5	4
8	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
9	A quantum chemical study of the effect of phosphine ligand on the structure of the Mn and Fe vinylidene binuclear complex. Journal of Structural Chemistry, 2016, 57, 267-274.	1.0	2
10	Theoretical Study of the Methanol Dehydrogenation on Platinum Nanocluster. Journal of Siberian Federal University: Chemistry, 2016, 9, 430-442.	0.7	3
11	Density Functional Calculation of Dioxygen Adsorption at Complexes of Ceria Nanoparticle with Atoms, Trimers and Tetramers of Silver. Journal of Siberian Federal University: Chemistry, 2016, 9, 281-295.	0.7	1
12	Trinuclear tantalum clusters grafted to hydroxylated silica surfaces: A density-functional embedded-cluster study. Kinetics and Catalysis, 2015, 56, 631-639.	1.0	1
13	Interaction of silica-supported small silver clusters with molecular oxygen. A computational study. Surface Science, 2014, 630, 265-272.	1.9	12
14	Reverse hydrogen spillover on and hydrogenation of supported metal clusters: insights from computational model studies. Physical Chemistry Chemical Physics, 2012, 14, 5879.	2.8	18
15	Cationic Zinc Species in ZSM-5 Zeolites: Structure and Stability from Embedded Cluster Modeling. Soft Materials, 2012, 10, 216-234.	1.7	3
16	Vinylidene carbonylation at a manganeseâ€“iron complex: A density functional study of mechanism. Journal of Organometallic Chemistry, 2011, 696, 3445-3453.	1.8	7
17	Small silver clusters at paramagnetic defects of silica surfaces. Surface Science, 2010, 604, 1705-1712.	1.9	8
18	Small gold species at hydroxylated alumina surfaces. A computational study using embedded-cluster models of Î±-Al2O3(0001). Chemical Physics Letters, 2010, 494, 243-248.	2.6	3

#	Article	IF	Citations
19	Simulation of heterogeneous catalysts and catalytic processes using the density functional method. Kinetics and Catalysis, 2010, 51, 832-842.	1.0	4
20	Effect of the size of the quantum region in a hybrid embedded-cluster scheme for zeolite systems. Chemical Physics, 2009, 363, 33-41.	1.9	16
21	Reverse Hydrogen Spillover onto Zeolite-Supported Metal Clusters:â€‰ An Embedded Cluster Density Functional Study of Models M₆(M = Rh, Ir, or Au). Journal of Physical Chemistry C, 2007, 111, 12340-12351.	3.1	57
22	First Hybrid Embedding Scheme for Polar Covalent Materials Using an Extended Border Region To Minimize Boundary Effects on the Quantum Region. Journal of Chemical Theory and Computation, 2007, 3, 2290-2300.	5.3	21
23	Modeling metal adsorption at amorphous silica: Gold atoms and dimers as example. Chemical Physics Letters, 2007, 444, 280-286.	2.6	22
24	Complexes of ortho-nitrophenols with aluminum bromide in nonaqueous solutions. Russian Journal of Applied Chemistry, 2007, 80, 887-890.	0.5	1
25	Correlation between structure and spectral characteristics of rhodium(I) chelate dicarbonyl complexes and their electron. Journal of Structural Chemistry, 2005, 46, 220-229.	1.0	15
26	Comparison of All Sites for Ti Substitution in Zeolite TS-1 by an Accurate Embedded-Cluster Method. Journal of Physical Chemistry B, 2005, 109, 24304-24310.	2.6	50
27	Effects of the Aluminum Content of a Zeolite Framework:â€‰ A DFT/MM Hybrid Approach Based on Cluster Models Embedded in an Elastic Polarizable Environment. Journal of Chemical Theory and Computation, 2005, 1, 459-471.	5.3	36
28	Elastic Polarizable Environment Cluster Embedding Approach for Covalent Oxides and Zeolites Based on a Density Functional Method. Journal of Physical Chemistry B, 2003, 107, 2228-2241.	2.6	73
29	Methanol Carbonylation Catalyzed by the Anion of the Complex Dicarbonyldiiodorhodium(I). A Density Functional Study of the Catalytic Cycle. Organometallics, 2001, 20, 1161-1174.	2.3	36
30	Reactions of Phenols with Lewis Acids: XX. Tautomerism of Naphthols. Russian Journal of Organic Chemistry, 2001, 37, 1270-1272.	0.8	1
31	Interactions of Phenols with Lewis Acids: XVIII. Tautomerism of Methylated Phenols. Russian Journal of Organic Chemistry, 2001, 37, 1114-1116.	0.8	1