

# Alexei M Shor

## List of Publications by Year in descending order

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31  
papers

464  
citations

759233

12  
h-index

713466

21  
g-index

33  
all docs

33  
docs citations

33  
times ranked

606  
citing authors

#	ARTICLE	IF	CITATIONS
1	Elastic Polarizable Environment Cluster Embedding Approach for Covalent Oxides and Zeolites Based on a Density Functional Method. <i>Journal of Physical Chemistry B</i> , 2003, 107, 2228-2241.	2.6	73
2	Reverse Hydrogen Spillover onto Zeolite-Supported Metal Clusters: An Embedded Cluster Density Functional Study of Models $M_6$ ( $M = Rh, Ir, \text{ or } Au$ ). <i>Journal of Physical Chemistry C</i> , 2007, 111, 12340-12351.	3.1	57
3	Comparison of All Sites for Ti Substitution in Zeolite TS-1 by an Accurate Embedded-Cluster Method. <i>Journal of Physical Chemistry B</i> , 2005, 109, 24304-24310.	2.6	50
4	Size-Dependence of the Adsorption Energy of CO on Pt Nanoparticles: Tracing Two Intersecting Trends by DFT Calculations. <i>Journal of Physical Chemistry C</i> , 2017, 121, 17371-17377.	3.1	39
5	Methanol Carbonylation Catalyzed by the Anion of the Complex Dicarbonyldiiodorhodium(I). A Density Functional Study of the Catalytic Cycle. <i>Organometallics</i> , 2001, 20, 1161-1174.	2.3	36
6	Effects of the Aluminum Content of a Zeolite Framework: A DFT/MM Hybrid Approach Based on Cluster Models Embedded in an Elastic Polarizable Environment. <i>Journal of Chemical Theory and Computation</i> , 2005, 1, 459-471.	5.3	36
7	Modeling metal adsorption at amorphous silica: Gold atoms and dimers as example. <i>Chemical Physics Letters</i> , 2007, 444, 280-286.	2.6	22
8	First Hybrid Embedding Scheme for Polar Covalent Materials Using an Extended Border Region To Minimize Boundary Effects on the Quantum Region. <i>Journal of Chemical Theory and Computation</i> , 2007, 3, 2290-2300.	5.3	21
9	Reverse hydrogen spillover on and hydrogenation of supported metal clusters: insights from computational model studies. <i>Physical Chemistry Chemical Physics</i> , 2012, 14, 5879.	2.8	18
10	Effect of the size of the quantum region in a hybrid embedded-cluster scheme for zeolite systems. <i>Chemical Physics</i> , 2009, 363, 33-41.	1.9	16
11	Correlation between structure and spectral characteristics of rhodium(I) chelate dicarbonyl complexes and their electron. <i>Journal of Structural Chemistry</i> , 2005, 46, 220-229.	1.0	15
12	Interaction of silica-supported small silver clusters with molecular oxygen. A computational study. <i>Surface Science</i> , 2014, 630, 265-272.	1.9	12
13	What Changes on the Inverse Catalyst? Insights from CO Oxidation on Au-Supported Ceria Nanoparticles Using Ab Initio Molecular Dynamics. <i>ACS Catalysis</i> , 2020, 10, 3164-3174.	11.2	11
14	Small silver clusters at paramagnetic defects of silica surfaces. <i>Surface Science</i> , 2010, 604, 1705-1712.	1.9	8
15	Silver atom, trimer and tetramer species supported on a ceria nanoparticle: A density functional study. <i>Surface Science</i> , 2019, 681, 38-46.	1.9	8
16	Vinylidene carbonylation at a manganese-iron complex: A density functional study of mechanism. <i>Journal of Organometallic Chemistry</i> , 2011, 696, 3445-3453.	1.8	7
17	Simulation of heterogeneous catalysts and catalytic processes using the density functional method. <i>Kinetics and Catalysis</i> , 2010, 51, 832-842.	1.0	4
18	Theoretical study of O <sub>2</sub> interaction with subnanometer-sized Ag clusters supported on defective SiO <sub>2</sub> surface. <i>Computational and Theoretical Chemistry</i> , 2018, 1144, 56-65.	2.5	4

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19	Small gold species at hydroxylated alumina surfaces. A computational study using embedded-cluster models of $\gamma$ -Al <sub>2</sub> O <sub>3</sub> (0001). <i>Chemical Physics Letters</i> , 2010, 494, 243-248.	2.6	3
20	Cationic Zinc Species in ZSM-5 Zeolites: Structure and Stability from Embedded Cluster Modeling. <i>Soft Materials</i> , 2012, 10, 216-234.	1.7	3
21	Hydration Structure and Hydrolysis of U(IV) and Np(IV) Ions: A Comparative Density Functional Study Using a Modified Continuum Solvation Approach. <i>Journal of Physical Chemistry A</i> , 2020, 124, 3805-3814.	2.5	3
22	Theoretical Study of the Methanol Dehydrogenation on Platinum Nanocluster. <i>Journal of Siberian Federal University: Chemistry</i> , 2016, 9, 430-442.	0.7	3
23	Size and structure effects on platinum nanocatalysts: theoretical insights from methanol dehydrogenation. <i>Nanoscale</i> , 2022, 14, 4145-4155.	5.6	3
24	A quantum chemical study of the effect of phosphine ligand on the structure of the Mn and Fe vinylidene binuclear complex. <i>Journal of Structural Chemistry</i> , 2016, 57, 267-274.	1.0	2
25	Manganese "gold" manganese complex with vinylidene and acetylide units. <i>Dalton Transactions</i> , 2020, 49, 17527-17531.	3.3	2
26	Adsorption and Oxidation of CO on Ceria Nanoparticles Exposing Single-Atom Pd and Ag: A DFT Modelling. <i>Materials</i> , 2021, 14, 6888.	2.9	2
27	Reactions of Phenols with Lewis Acids: XX. Tautomerism of Naphthols. <i>Russian Journal of Organic Chemistry</i> , 2001, 37, 1270-1272.	0.8	1
28	Interactions of Phenols with Lewis Acids: XVIII. Tautomerism of Methylated Phenols. <i>Russian Journal of Organic Chemistry</i> , 2001, 37, 1114-1116.	0.8	1
29	Complexes of ortho-nitrophenols with aluminum bromide in nonaqueous solutions. <i>Russian Journal of Applied Chemistry</i> , 2007, 80, 887-890.	0.5	1
30	Trinuclear tantalum clusters grafted to hydroxylated silica surfaces: A density-functional embedded-cluster study. <i>Kinetics and Catalysis</i> , 2015, 56, 631-639.	1.0	1
31	Density Functional Calculation of Dioxygen Adsorption at Complexes of Ceria Nanoparticle with Atoms, Trimers and Tetramers of Silver. <i>Journal of Siberian Federal University: Chemistry</i> , 2016, 9, 281-295.	0.7	1