Hristiyan A Aleksandrov

List of Publications by Year
in descending order

79 papers	2,149 citations	201385 27 h-index	253896 43 g-index
81 all docs	81 docs citations	81 times ranked	2625 citing authors

#	Article	IF	Citations
1	One-pot synthesis of silanol-free nanosized MFIÂzeolite. Nature Materials, 2017, 16, 1010-1015.	13.3	135
2	Achieving Atomic Dispersion of Highly Loaded Transition Metals in Smallâ€Pore Zeolite SSZâ€13: Highâ€Capacity and Highâ€Efficiency Lowâ€Temperature CO and Passive NO_x Adsorbers. Angewandte Chemie - International Edition, 2018, 57, 16672-16677.	7.2	129
3	Can the state of platinum species be unambiguously determined by the stretching frequency of an adsorbed CO probe molecule?. Physical Chemistry Chemical Physics, 2016, 18, 22108-22121.	1.3	113
4	Water Chemistry on Model Ceria and Pt/Ceria Catalysts. Journal of Physical Chemistry C, 2012, 116, 12103-12113.	1.5	108
5	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
6	A DFT study of oxygen dissociation on platinum based nanoparticles. Nanoscale, 2014, 6, 1153-1165.	2.8	74
7	How Absorbed Hydrogen Affects the Catalytic Activity of Transition Metals. Angewandte Chemie - International Edition, 2014, 53, 13371-13375.	7.2	73
8	Stabilization of Super Electrophilic Pd⁺² Cations in Small-Pore SSZ-13 Zeolite. Journal of Physical Chemistry C, 2020, 124, 309-321.	1.5	67
9	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
10	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
11	Decomposition of ethylene on transition metal surfaces M(111). A comparative DFT study of model reactions for M=Pd, Pt, Rh, Ni. Journal of Molecular Catalysis A, 2011, 344, 37-46.	4.8	52
12	Stabilization of Small Platinum Nanoparticles on Ptâ€“CeO₂Thin Film Electrocatalysts During Methanol Oxidation. Journal of Physical Chemistry C, 2016, 120, 19723-19736.	1.5	50
13	Transformations of Ethylene on the Pd(111) Surface: A Density Functional Study. Journal of Physical Chemistry C, 2010, 114, 17683-17692.	1.5	47
14	FTIR and density functional study of NO interaction with reduced ceria: Identification of N3â˜ and NO2â˜ as new intermediates in NO conversion. Applied Catalysis B: Environmental, 2015, 176-177, 107-119.	10.8	43
15	Effect of MgO(100) support on structure and properties of Pd and Pt nanoparticles with 49-155 atoms. Journal of Chemical Physics, 2013, 139, 084701.	1.2	41
16	O2 Dissociation on M@Pt Coreâ€“Shell Particles for 3d, 4d, and 5d Transition Metals. Journal of Physical Chemistry C, 2015, 119, 11031-11041.	1.5	37
17	The structure and stability of reduced and oxidized mononuclear platinum species on nanostructured ceria from density functional modeling. Physical Chemistry Chemical Physics, 2015, 17, 14551-14560.	1.3	37
18	Study of active surface centers of Pt/CeO2 catalysts prepared using radio-frequency plasma sputtering technique. Surface Science, 2019, 679, 273-283.	0.8	37

#	Article	IF	Citations
19	New method for preparation of delivery systems of poorly soluble drugs on the basis of functionalized mesoporous MCM-41 nanoparticles. Microporous and Mesoporous Materials, 2014, 198, 247-255.	2.2	35
20	Achieving Atomic Dispersion of Highly Loaded Transition Metals in Smallâ€Pore Zeolite SSZâ€13: Highâ€Capacity and Highâ€Efficiency Lowâ€Temperature CO and Passive NO‹sub›‹i›x‹/i›‹/sub› Adsorbers. Angewandte Chemie, 2018, 130, 16914-16919.	1.6	34
21	Adsorbed and Subsurface Absorbed Hydrogen Atoms on Bare and MgO(100)-Supported Pd and Pt Nanoparticles. Journal of Physical Chemistry C, 2014, 118, 15242-15250.	1.5	33
22	Complex H-bonded silanol network in zeolites revealed by IR and NMR spectroscopy combined with DFT calculations. Journal of Materials Chemistry A, 2021, 9, 27347-27352.	5.2	33
23	Effect of Si/Al Ratio and Rh Precursor Used on the Synthesis of HY Zeolite-Supported Rhodium Carbonyl Hydride Complexes. Journal of Physical Chemistry C, 2015, 119, 17166-17181.	1.5	32
24	Subsurface Carbon: A General Feature of Noble Metals. Angewandte Chemie - International Edition, 2019, 58, 1744-1748.	7.2	31
25	Species formed during NO adsorption and NOâ€¯+â€¯O 2 co-adsorption on ceria: A combined FTIR and DFT study. Molecular Catalysis, 2018, 451, 114-124.	1.0	30
26	Heterolytic dissociation and recombination of H2 over Zn,H-ZSM-5 zeolitesâ€”A density functional model study. Journal of Molecular Catalysis A, 2006, 256, 149-155.	4.8	29
27	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
28	Tuning the Surface Chemistry of Pd by Atomic C and H: A Microscopic Picture. Chemistry - A European Journal, 2013, 19, 1335-1345.	1.7	28
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.	1.3	27
30	Modified mesoporous silica nanoparticles coated by polymer complex as novel curcumin delivery carriers. Journal of Drug Delivery Science and Technology, 2019, 49, 700-712.	1.4	27
31	Framework Stability of Heteroatom-Substituted Forms of Extra-Large-Pore Ge-Silicate Molecular Sieves: The Case of ITQ-44. Chemistry of Materials, 2012, 24, 2509-2518.	3.2	26
32	Synthesis, Modeling, and Catalytic Properties of HY Zeolite-Supported Rhodium Dinitrosyl Complexes. ACS Catalysis, 2017, 7, 5965-5982.	5.5	26
33	Energetic Stability of Absorbed H in Pd and Pt Nanoparticles in a More Realistic Environment. Journal of Physical Chemistry C, 2015, 119, 5180-5186.	1.5	25
34	Paraquat adsorption on NaY zeolite at various Si/Al ratios: A combined experimental and computational study. Materials Chemistry and Physics, 2019, 238, 121824.	2.0	25
35	DFT studies of oxygen dissociation on the 116-atom platinum truncated octahedron particle. Physical Chemistry Chemical Physics, 2014, 16, 26539-26545.	1.3	23
36	Theoretical investigation of ethane dehydrogenation on cationic Zn species in ZSM-5 zeolitesâ€”The second Al center in vicinity of the cation is essential for the accomplishment of the complete catalytic cycle. Catalysis Today, 2010, 152, 78-87.	2.2	22

#	Article	IF	Citations
37	Experimental and theoretical study of quercetin complexes formed on pure silica and Zn-modified mesoporous MCM-41 and SBA-16 materials. Microporous and Mesoporous Materials, 2016, 228, 256-265.	2.2	21
38	Amino-modified KIT-6 mesoporous silica/polymer composites for quercetin delivery: Experimental and theoretical approaches. Microporous and Mesoporous Materials, 2018, 270, 40-47.	2.2	18
39	Unlocking the potential of hidden sites in FAUJASITE: new insights in a proton transfer mechanism. Angewandte Chemie - International Edition, 2021, 60, 26702-26709.	7.2	17
40	Effect of Si/Al Ratio on the Nature and Reactivity of HY Zeolite-Supported Rhodium Dicarbonyl Complexes. Journal of Physical Chemistry C, 2014, 118, 26772-26788.	1.5	16
41	Hydrophobic Tungsten-Containing MFI-Type Zeolite Films for Exhaust Gas Detection. ACS Applied Materials & Interfaces, 2019, 11, 12914-12919.	4.0	16
42	Precise Identification of the Infrared Bands of the Polycarbonyl Complexes on Niâ€“MOR Zeolite by12C16Oâ€“13C18O Coadsorption and Computational Modeling. Journal of Physical Chemistry C, 2012, 116, 22823-22831.	1.5	15
43	Elucidation of the higher coking resistance of small versus large nickel nanoparticles in methane dry reforming via computational modeling. Catalysis Science and Technology, 2017, 7, 3339-3347.	2.1	15
44	Structural transformations and adsorption properties of PtNi nanoalloy thin film electrocatalysts prepared by magnetron co-sputtering. Electrochimica Acta, 2017, 251, 427-441.	2.6	15
45	Interaction of Graphene with Out-of-Plane Aromatic Hydrocarbons. Journal of Physical Chemistry C, 2019, 123, 21448-21456.	1.5	14
46	Unraveling the Effect of Silanol Defects on the Insertion of Single-Site Mo in the MFI Zeolite Framework. Inorganic Chemistry, 2022, 61, 1418-1425.	1.9	14
47	Unusual Carbonylâ^'Nitrosyl Complexes of Rh2+in Rhâ^'ZSM-5:â€‰ A Combined FTIR Spectroscopy and Computational Study. Journal of Physical Chemistry C, 2007, 111, 10412-10418.	1.5	13
48	Formation of N₃^{â^'} during interaction of NO with reduced ceria. Chemical Communications, 2015, 51, 5668-5671.	2.2	12
49	Decomposition behavior of platinum clusters supported on ceria and Î³-alumina in the presence of carbon monoxide. Catalysis Science and Technology, 2017, 7, 734-742.	2.1	12
50	Room-Temperature Ethene Hydrogenation Activity of Transition-Metal-Free HY Zeolites. ACS Catalysis, 2019, 9, 839-847.	5.5	12
51	Chemical ordering in Ptâ€“Au, Ptâ€“Ag and Ptâ€“Cu nanoparticles from density functional calculations using a topological approach. Materials Advances, 2021, 2, 6589-6602.	2.6	12
52	Influence of the adsorption of CO on the electronic structure of platinum clusters and nanowires deposited on CeO2(111) and Î³-Al2O3(001) surfaces. Catalysis Today, 2020, 357, 442-452.	2.2	11
53	Inhibition of Palm Oil Oxidation by Zeolite Nanocrystals. Journal of Agricultural and Food Chemistry, 2015, 63, 4655-4663.	2.4	10
54	Characterization and temperature evolution of iron-containing species in HZSM-5 zeolite prepared from different iron sources. Journal of Porous Materials, 2019, 26, 1227-1240.	1.3	10

#	Article	IF	Citations
55	Impurity Atoms on Small Transition Metal Clusters. Insights from Density Functional Model Studies. Topics in Catalysis, 2011, 54, 363-377.	1.3	8
56	Verapamil delivery systems on the basis of mesoporous ZSM-5/KIT-6 and ZSM-5/SBA-15 polymer nanocomposites as a potential tool to overcome MDR in cancer cells. European Journal of Pharmaceutics and Biopharmaceutics, 2019, 142, 460-472.	2.0	8
57	Tamoxifen Delivery System Based on PEGylated Magnetic MCM-41 Silica. Molecules, 2020, 25, 5129.	1.7	8
58	Surface chemistry of reduced graphene oxide: H-atom transfer reactions. Applied Surface Science, 2021, 567, 150815.	3.1	8
59	Biomimetic CO oxidation below â˜'100â€‰Â°C by a nitrate-containing metal-free microporous system. Nature Communications, 2021, 12, 6033.	5.8	8
60	Theoretical Investigation of the Coordination of N2Ligands to the Cluster Ni3. Journal of Physical Chemistry A, 2004, 108, 6127-6144.	1.1	7
61	Using density functional calculations to elucidate atomic ordering of Pd-Rh nanoparticles at sizes relevant for catalytic applications. Chinese Journal of Catalysis, 2019, 40, 1749-1757.	6.9	7
62	Relative stability and reducibility of CeO2 and Rh/CeO2 species on the surface and in the cavities of Î³-Al2O3: a periodic DFT study. Physical Chemistry Chemical Physics, 2015, 17, 22389-22401.	1.3	6
63	Subsurface Carbon: A General Feature of Noble Metals. Angewandte Chemie, 2019, 131, 1758-1762.	1.6	6
64	Preferential location of zirconium dopants in cerium dioxide nanoparticles and the effects of doping on their reducibility: a DFT study. Physical Chemistry Chemical Physics, 2020, 22, 26568-26582.	1.3	6
65	Design of PEG-modified magnetic nanoporous silica based miltefosine delivery system: Experimental and theoretical approaches. Microporous and Mesoporous Materials, 2021, 310, 110664.	2.2	6
66	Charting the Atomic C Interaction with Transition Metal Surfaces. ACS Catalysis, 2022, 12, 9256-9269.	5.5	6
67	Computational evaluation of the capability of transition metal exchanged zeolites for complete purification of hydrogen for fuel cell applications: the cheapest performs the best. Energy and Environmental Science, 2011, 4, 1879.	15.6	5
68	Structure and reducibility of yttrium-doped cerium dioxide nanoparticles and (111) surface. RSC Advances, 2018, 8, 33728-33741.	1.7	5
69	Key Role of aâ€Top CO on Terrace Sites of Metallic Pd Clusters for CO Oxidation. Chemistry - A European Journal, 2022, 28, .	1.7	5
70	Computational Modelling of Nanoporous Materials. , 2009, , 211-238.		4
71	Catalytic conversion of ethene to butadiene or hydrogenation to ethane on HY zeolite-supported rhodium complexes: Cooperative support/Rh-center route. Journal of Chemical Physics, 2021, 154, 184706.	1.2	4
72	Computational Modeling of Coordination Chemistry of Transition Metal Cations in Zeolites and in Metal-organic Frameworks. Current Physical Chemistry, 2012, 2, 189-199.	0.1	4

#	Article	IF	Citations
73	Unlocking the potential of hidden sites in FAUJASITE: new insights in a proton transfer mechanism. Angewandte Chemie, 0, , .	1.6	4
74	Defect Formation, T-Atom Substitution and Adsorption of Guest Molecules in MSE-Type Zeolite Frameworkâ€"DFT Modeling. Molecules, 2021, 26, 7296.	1.7	4
75	Cationic Zinc Species in ZSM-5 Zeolites: Structure and Stability from Embedded Cluster Modeling. Soft Materials, 2012, 10, 216-234.	0.8	3
76	Approaching complexity of alkyl hydrogenation on Pd via density-functional modelling. Physical Chemistry Chemical Physics, 2017, 19, 21514-21521.	1.3	3
77	RÃ¼cktitelbild: Achieving Atomic Dispersion of Highly Loaded Transition Metals in Smallâ€Pore Zeolite SSZâ€13: Highâ€Capacity and Highâ€Efficiency Lowâ€Temperature CO and Passive NO_x Adsorbers (Angew. Chem. 51/2018). Angewandte Chemie, 2018, 130, 17152-17152.	1.6	1
78	Band gap modulation of graphene on SiC. European Physical Journal B, 2018, 91, 1.	0.6	1
79	Computational Modeling of Coordination Chemistry of Transition Metal Cations in Zeolites and in Metal-organic Frameworks. Current Physical Chemistry, 2012, 2, 189-199.	0.1	0