Konstantin M Neyman

List of Publications by Year
in descending order

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184	11,732	22153 59	33894 99
papers	citations	h-index	g-index

195	195	195	9057
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	Support nanostructure boosts oxygen transfer to catalytically active platinum nanoparticles. Nature Materials, 2011, 10, 310-315.	27.5	748
2	First-principlesLDA+UandGGA+Ustudy of cerium oxides: Dependence on the effective U parameter. Physical Review B, 2007, 75, .	3.2	634
3	Counting electrons on supported nanoparticles. Nature Materials, 2016, 15, 284-288.	27.5	469
4	Maximum Nobleâ€Metal Efficiency in Catalytic Materials: Atomically Dispersed Surface Platinum. Angewandte Chemie - International Edition, 2014, 53, 10525-10530.	13.8	384
5	Reassignment of the Vibrational Spectra of Carbonates, Formates, and Related Surface Species on Ceria: A Combined Density Functional and Infrared Spectroscopy Investigation. Journal of Physical Chemistry C, 2011, 115, 23435-23454.	3.1	294
6	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
7	CO Adsorption on Pd Nanoparticles:Â Density Functional and Vibrational Spectroscopy Studies. Journal of Physical Chemistry B, 2003, 107, 255-264.	2.6	262
8	Dramatic reduction of the oxygen vacancy formation energy in ceria particles: a possible key to their remarkable reactivity at the nanoscale. Journal of Materials Chemistry, 2010, 20, 10535.	6.7	192
9	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
10	Greatly facilitated oxygen vacancy formation in ceria nanocrystallites. Chemical Communications, 2010, 46, 5936.	4.1	160
11	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
12	The role of metal/oxide interfaces for long-range metal particle activation during CO oxidation. Nature Materials, 2018, 17, 519-522.	27.5	136
13	CH3O Decomposition on PdZn(111), Pd(111), and Cu(111). A Theoretical Study. Langmuir, 2004, 20, 8068-8077.	3.5	133
14	Methane Activation by Platinum: Critical Role of Edge and Corner Sites of Metal Nanoparticles. Chemistry - A European Journal, 2010, 16, 6530-6539.	3.3	126
15	Density functional studies of model cerium oxide nanoparticles. Physical Chemistry Chemical Physics, 2008, 10, 5730.	2.8	125
16	On the Promoting Role of Ag in Selective Hydrogenation Reactions over Pdâ^'Ag Bimetallic Catalysts:â€‰ A Theoretical Study. Journal of Physical Chemistry C, 2007, 111, 6852-6856.	3.1	121
17	Silver residues as a possible key to a remarkable oxidative catalytic activity of nanoporous gold. Physical Chemistry Chemical Physics, 2011, 13, 4529.	2.8	121
18	Cluster embedding in an elastic polarizable environment: Density functional study of Pd atoms adsorbed at oxygen vacancies of MgO(001). Journal of Chemical Physics, 2001, 115, 8157-8171.	3.0	116

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19	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.	2.8	113
20	Surface structure and stability of PdZn and PtZn alloys:â€ƒDensity-functional slab model studies. Physical Review B, 2003, 68, .	3.2	108
21	Water Chemistry on Model Ceria and Pt/Ceria Catalysts. Journal of Physical Chemistry C, 2012, 116, 12103-12113.	3.1	108
22	Formation of Superoxide Anions on Ceria Nanoparticles by Interaction of Molecular Oxygen with Ce³⁺ Sites. Journal of Physical Chemistry C, 2011, 115, 5817-5822.	3.1	107
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	Approaching nanoscale oxides: models and theoretical methods. Chemical Society Reviews, 2009, 38, 2657.	38.1	105
25	N2 and CO molecules as probes of zeolite acidity: an infrared spectroscopy and density functional investigation. Catalysis Letters, 1995, 31, 273-285.	2.6	104
26	Adsorption and reaction of methanol on supported palladium catalysts: microscopic-level studies from ultrahigh vacuum to ambient pressure conditions. Physical Chemistry Chemical Physics, 2007, 9, 3541-3558.	2.8	100
27	Understanding Ceria Nanoparticles from First-Principles Calculations. Journal of Physical Chemistry C, 2007, 111, 10142-10145.	3.1	99
28	Atomically Dispersed Pd, Ni, and Pt Species in Ceria-Based Catalysts: Principal Differences in Stability and Reactivity. Journal of Physical Chemistry C, 2016, 120, 9852-9862.	3.1	99
29	CO Interaction with Alkali Metal Cations in Zeolites:Â A Density Functional Model Cluster Study. Journal of Physical Chemistry B, 1997, 101, 9292-9298.	2.6	97
30	Comparative Theoretical Study of Formaldehyde Decomposition on PdZn, Cu, and Pd Surfaces. Journal of Physical Chemistry B, 2006, 110, 14890-14897.	2.6	96
31	Microscopic models of PdZn alloy catalysts: structure and reactivity in methanol decomposition. Physical Chemistry Chemical Physics, 2007, 9, 3470-3482.	2.8	96
32	Electronic properties of thin Zn layers on Pd(111) during growth and alloying. Surface Science, 2006, 600, 78-94.	1.9	95
33	Towards stable single-atom catalysts: strong binding of atomically dispersed transition metals on the surface of nanostructured ceria. Catalysis Science and Technology, 2016, 6, 6806-6813.	4.1	92
34	Hydrogen Diffusion into Palladium Nanoparticles: Pivotal Promotion by Carbon. Angewandte Chemie - International Edition, 2010, 49, 4743-4746.	13.8	91
35	Effects of deposited Pt particles on the reducibility of CeO2(111). Physical Chemistry Chemical Physics, 2011, 13, 11384.	2.8	89
36	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

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37	Adsorption of d-metal atoms on the regular MgO(001) surface: Density functional study of cluster models embedded in an elastic polarizable environment. Applied Physics A: Materials Science and Processing, 2004, 78, 823-828.	2.3	84
38	Oxide-based nanomaterials for fuel cell catalysis: the interplay between supported single Pt atoms and particles. Catalysis Science and Technology, 2017, 7, 4315-4345.	4.1	84
39	Pd and Ag dimers and tetramers adsorbed at the MgO(001) surface: a density functional study. Physical Chemistry Chemical Physics, 1999, 1, 4655-4661.	2.8	83
40	CO oxidation activity of Pt/CeO2 catalysts below 0 Â°C: platinum loading effects. Applied Catalysis B: Environmental, 2021, 286, 119931.	20.2	83
41	CO bonding and vibrational modes on a perfect MgO(001) surface: LCGTO-LDF model cluster investigation. Chemical Physics, 1992, 168, 267-280.	1.9	81
42	Adsorption of CO molecules on a MgO(001) surface. Model cluster density functional study employing a gradient-corrected potential. Chemical Physics Letters, 1995, 246, 546-554.	2.6	80
43	Single d-Metal Atoms on Fsand Fs+Defects of MgO(001):Â A Theoretical Study across the Periodic Table. Journal of the American Chemical Society, 2005, 127, 11652-11660.	13.7	80
44	Density functional study of M4 clusters (M=Cu, Ag, Ni, Pd) deposited on the regular MgO(001) surface. Chemical Physics Letters, 1999, 299, 603-612.	2.6	77
45	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
46	Faujasite-Supported Ir4Clusters:Â A Density Functional Model Study of Metalâ^'Zeolite Interactions. Journal of Physical Chemistry B, 1999, 103, 5311-5319.	2.6	75
47	A DFT study of oxygen dissociation on platinum based nanoparticles. Nanoscale, 2014, 6, 1153-1165.	5.6	74
48	How Absorbed Hydrogen Affects the Catalytic Activity of Transition Metals. Angewandte Chemie - International Edition, 2014, 53, 13371-13375.	13.8	73
49	Calculation of Electronic g-Tensors Using a Relativistic Density Functional Douglasâ^'Kroll Method. Journal of Physical Chemistry A, 2002, 106, 5022-5030.	2.5	71
50	Edge sites as a gate for subsurface carbon in palladium nanoparticles. Journal of Catalysis, 2009, 266, 59-63.	6.2	71
51	Adsorption, Oxidation State, and Diffusion of Pt Atoms on the CeO₂(111) Surface. Journal of Physical Chemistry C, 2010, 114, 14202-14207.	3.1	71
52	How to determine accurate chemical ordering in several nanometer large bimetallic crystallites from electronic structure calculations. Chemical Science, 2015, 6, 3868-3880.	7.4	70
53	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
54	Density Functional Study of N2 Activation by Molybdenum(III) Complexes. Unusually Strong Relativistic Effects in 4d Metal Compounds. Organometallics, 1997, 16, 995-1000.	2.3	67

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55	Bonding and vibration of CO molecules adsorbed on low-coordinated surface sites of MgO: a LCGTO-LDF cluster investigation. Surface Science, 1993, 297, 223-234.	1.9	65
56	Theoretical aspects of heterogeneous catalysis: Applications of density functional methods. Catalysis Today, 2005, 105, 2-16.	4.4	65
57	On the difficulties of present theoretical models to predict the oxidation state of atomic Au adsorbed on regular sites of CeO[sub 2](111). Journal of Chemical Physics, 2009, 131, 094702.	3.0	64
58	Modeling Ceria-Based Nanomaterials for Catalysis and Related Applications. Catalysis Letters, 2016, 146, 2053-2080.	2.6	63
59	FTIR Spectroscopic and Density Functional Model Cluster Studies of Methane Adsorption on MgO. Journal of Physical Chemistry B, 1998, 102, 4548-4555.	2.6	61
60	Density functional studies of coinage metal nanoparticles: scalability of their properties to bulk. Theoretical Chemistry Accounts, 2008, 120, 565-573.	1.4	61
61	Formation of One-Dimensional Electronic States along the Step Edges of CeO₂(111). ACS Nano, 2012, 6, 1126-1133.	14.6	61
62	Reactivity of atomically dispersed Pt²⁺ species towards H₂: model Ptâ€“CeO₂ fuel cell catalyst. Physical Chemistry Chemical Physics, 2016, 18, 7672-7679.	2.8	61
63	Computational Study of Model Pdâ^'Zn Nanoclusters and Their Adsorption Complexes with CO Molecules. Journal of Physical Chemistry B, 2004, 108, 5424-5430.	2.6	59
64	Stabilization of Au at edges of bimetallic PdAu nanocrystallites. Physical Chemistry Chemical Physics, 2010, 12, 5094.	2.8	57
65	Density Functional Studies of Alkali-Exchanged Zeolites. Cation Location at Six-Rings of Different Aluminum Content. Journal of Physical Chemistry B, 1999, 103, 7920-7928.	2.6	55
66	Theoretical study of segregation of Zn and Pd in Pdâ€“Zn alloys. Surface Science, 2004, 548, 291-300.	1.9	54
67	Density Functional Theory Study of the Adsorption of Au Atom on Cerium Oxide: Effect of Low-Coordinated Surface Sites. Journal of Physical Chemistry C, 2009, 113, 4948-4954.	3.1	54
68	A Surface Site as Polydentate Ligand of a Metal Complex:â€‰ Density Functional Studies of Rhenium Subcarbonyls Supported on Magnesium Oxide. Journal of the American Chemical Society, 1999, 121, 4522-4523.	13.7	53
69	On the Mechanism of Formation of Metal Nanowires by Selfâ€Assembly. Angewandte Chemie - International Edition, 2007, 46, 7094-7097.	13.8	53
70	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.	2.3	52
71	High efficiency of Pt2+- CeO2 novel thin film catalyst as anode for proton exchange membrane fuel cells. Applied Catalysis B: Environmental, 2016, 197, 262-270.	20.2	52
72	Exploring Ce3+/Ce4+ cation ordering in reduced ceria nanoparticles using interionic-potential and density-functional calculations. Journal of Chemical Physics, 2009, 131, 064701.	3.0	50

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73	Stabilization of Small Platinum Nanoparticles on Ptâ€“CeO₂Thin Film Electrocatalysts During Methanol Oxidation. Journal of Physical Chemistry C, 2016, 120, 19723-19736.	3.1	50
74	Acidic properties of [Al], [Ga] and [Fe] isomorphously substituted zeolites. Density functional model cluster study of the complexes with a probe CO molecule. Chemical Physics Letters, 1995, 240, 547-552.	2.6	49
75	Bonding and vibrations of CO molecules adsorbed at transition metal impurity sites on the MgO (001) surface. A density functional model cluster study. Chemical Physics, 1993, 177, 561-570.	1.9	48
76	Effect of Steps on the Decomposition of CH3O at PdZn Alloy Surfaces. Journal of Physical Chemistry B, 2005, 109, 4568-4574.	2.6	48
77	Surface composition changes of CuNi-ZrO2 during methane decomposition: An operando NAP-XPS and density functional study. Catalysis Today, 2017, 283, 134-143.	4.4	48
78	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
79	Adsorption of isolated Cu, Ni and Pd atoms on various sites of MgO(001): Density functional studies. Nuovo Cimento Della Societa Italiana Di Fisica D - Condensed Matter, Atomic, Molecular and Chemical Physics, Biophysics, 1997, 19, 1743-1748.	0.4	46
80	Ligand-Free Osmium Clusters Supported on MgO. A Density Functional Study. Langmuir, 2000, 16, 2736-2743.	3.5	46
81	Adsorption and oxidation of NO on Au(111) surface: Density functional studies. Chemical Physics Letters, 2006, 422, 412-416.	2.6	45
82	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
83	Carbon on Platinum Substrates: From Carbidic to Graphitic Phases on the (111) Surface and on Nanoparticles. Journal of Physical Chemistry A, 2009, 113, 11963-11973.	2.5	44
84	Unravelling Morphological and Topological Energy Contributions of Metal Nanoparticles. Nanomaterials, 2022, 12, 17.	4.1	44
85	Prediction of Alternative Structures of the Molybdenum Site in the Xanthine Oxidase-Related Aldehyde Oxido Reductase. Journal of the American Chemical Society, 1997, 119, 3159-3160.	13.7	43
86	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
87	CO adsorption on the (001) surface of MgO: a comparison of Hartree-Fock and local density functional results. Journal of Electron Spectroscopy and Related Phenomena, 1994, 69, 13-21.	1.7	42
88	Structural features of the NO/Ru(001) adsorption complexes: A linear combination of Gaussianâ€type orbitals local density functional model cluster analysis of highâ€resolution electron energy loss spectroscopy data. Journal of Chemical Physics, 1994, 100, 2310-2321.	3.0	41
89	A Combined Density-Functional and IRAS Study on the Interaction of NO with Pd Nanoparticles: Identifying New Adsorption Sites with Novel Properties. Journal of Physical Chemistry C, 2008, 112, 16539-16549.	3.1	41
90	Density Functional Calculations of Pd Nanoparticles Using a Plane-Wave Method. Journal of Physical Chemistry A, 2008, 112, 8911-8915.	2.5	41

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91	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.	3.0	41
92	Effects of electron transfer in model catalysts composed of Pt nanoparticles on CeO2(1 1 1) surface. Journal of Catalysis, 2016, 344, 507-514.	6.2	41
93	Adsorption of Pd and Pt atoms on Î±-Al2O3(): density functional study of cluster models embedded in an elastic polarizable environment. Surface Science, 2003, 525, 173-183.	1.9	40
94	Atomic and Electronic Structure of Cerium Oxide Stepped Model Surfaces. Journal of Physical Chemistry C, 2008, 112, 17643-17651.	3.1	40
95	Density Functional Modeling of the Interactions of Platinum Clusters with CeO₂ Nanoparticles of Different Size. Journal of Physical Chemistry C, 2011, 115, 16081-16086.	3.1	40
96	Geometric Arrangement of Components in Bimetallic PdZn/Pd(111) Surfaces Modified by CO Adsorption: A Combined Study by Density Functional Calculations, Polarization-Modulated Infrared Reflection Absorption Spectroscopy, and Temperature-Programmed Desorption. Journal of Physical Chemistry C, 2012, 116, 18768-18778.	3.1	40
97	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
98	Modification of structural and chemisorption properties of small palladium clusters supported on the MgO(001) surface from density functional calculations. Applied Catalysis A: General, 2000, 191, 3-13.	4.3	39
99	Absolute Surface Step Energies: Accurate Theoretical Methods Applied to Ceria Nanoislands. Journal of Physical Chemistry Letters, 2012, 3, 1956-1961.	4.6	38
100	Insights from methane decomposition on nanostructured palladium. Journal of Catalysis, 2016, 337, 111-121.	6.2	38
101	Steric Effects on Dinitrogen Cleavage by Three-Coordinate Molybdenum(III) Complexes:â€‰ A Molecular Mechanics Study. Inorganic Chemistry, 1997, 36, 3947-3951.	4.0	37
102	Comment on â€œFirst-principles determination of the bonding mechanism and adsorption energy for CO/MgO(001)â€•[Chem. Phys. Lett. 290 (1998) 255]. Chemical Physics Letters, 1999, 306, 202-204.	2.6	37
103	O2 Dissociation on M@Pt Coreâ€“Shell Particles for 3d, 4d, and 5d Transition Metals. Journal of Physical Chemistry C, 2015, 119, 11031-11041.	3.1	37
104	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.	2.8	37
105	Study of active surface centers of Pt/CeO2 catalysts prepared using radio-frequency plasma sputtering technique. Surface Science, 2019, 679, 273-283.	1.9	37
106	Small Platinum Clusters in Zeolites:Â A Density Functional Study of CO Adsorption on Electronically Modified Models. Journal of Physical Chemistry B, 1999, 103, 216-226.	2.6	36
107	Density-functional model cluster studies of EPR g tensors of Fs+ centers on the surface of MgO. Journal of Chemical Physics, 2006, 124, 044708.	3.0	36
108	Adsorption of carbon on Pd clusters of nanometer size: A first-principles theoretical study. Journal of Chemical Physics, 2005, 122, 174705.	3.0	33

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109	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
110	Oxygen vacancies in self-assemblies of ceria nanoparticles. Journal of Materials Chemistry A, 2014, 2, 18329-18338.	10.3	33
111	O vacancies on steps on the CeO2(111) surface. Physical Chemistry Chemical Physics, 2014, 16, 7823.	2.8	33
112	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.	3.1	33
113	Surface composition of magnetron sputtered Pt-Co thin film catalyst for proton exchange membrane fuel cells. Applied Surface Science, 2016, 365, 245-251.	6.1	33
114	Pd3 and Pt3 species on the Î±-Al2O3(0001) surface: cluster models embedded in an elastic polarizable environment. Chemical Physics Letters, 2003, 374, 487-495.	2.6	32
115	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.	0.4	32
116	Towards size-converged properties of model ceria nanoparticles: Monitoring by adsorbed CO using DFT +U approach. Chemical Physics Letters, 2008, 465, 106-109.	2.6	31
117	Lateral Interaction between Adsorbates at Ionic Surfaces: Theoretical Investigation of the CO Vibrational Frequency Shift at MgO(001). Zeitschrift Fur Elektrotechnik Und Elektrochemie, 1992, 96, 1711-1715.	0.9	30
118	Oxygen atoms on the (111) surface of coinage metals: On the chemical state of the adsorbate. Chemical Physics Letters, 2006, 429, 86-90.	2.6	30
119	Metal-doped ceria nanoparticles: stability and redox processes. Physical Chemistry Chemical Physics, 2017, 19, 21729-21738.	2.8	30
120	Density functional and infrared spectroscopy studies of bonding and vibrations of NH species adsorbed on the Ru(001) surface: a reassignment of the bending mode band. Surface Science, 1996, 369, 300-312.	1.9	29
121	Density functional study of methoxide decomposition on PdZn(100). Physical Chemistry Chemical Physics, 2004, 6, 4499-4504.	2.8	29
122	Versatile Optimization of Chemical Ordering in Bimetallic Nanoparticles. Journal of Physical Chemistry C, 2017, 121, 10803-10808.	3.1	29
123	A density functional study of CO adsorption on three- and five-coordinate Al in oxide systems. Catalysis Letters, 1996, 40, 183-188.	2.6	28
124	Title is missing!. Topics in Catalysis, 1999, 9, 153-161.	2.8	28
125	Catalysis from First Principles: Towards Accounting for the Effects of Nanostructuring. Topics in Catalysis, 2013, 56, 867-873.	2.8	28
126	Tuning the Surface Chemistry of Pd by Atomic C and H: A Microscopic Picture. Chemistry - A European Journal, 2013, 19, 1335-1345.	3.3	28

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127	Electronic and Geometric Structure of Bimetallic Clusters:Â Density Functional Calculations on [M4{Fe(CO)4}4]4-(M = Cu, Ag, Au) and [Ag13{Fe(CO)4}8]n-(n= 0â^'5). Inorganic Chemistry, 1996, 35, 7370-7376.	4.0	27
128	Adsorption Preference Determines Segregation Direction: A Shortcut to More Realistic Surface Models of Alloy Catalysts. ACS Catalysis, 2019, 9, 5011-5018.	11.2	27
129	Interaction of CO Molecules with Electron-Deficient Pt Atoms in Zeolites:Â A Density Functional Model Cluster Study. The Journal of Physical Chemistry, 1996, 100, 3482-3487.	2.9	26
130	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.	2.6	26
131	Irreversible structural dynamics on the surface of bimetallic PtNi alloy catalyst under alternating oxidizing and reducing environments. Applied Catalysis B: Environmental, 2020, 264, 118476.	20.2	26
132	Adsorption of acrolein on single-crystal surfaces of silver: Density functional studies. Chemical Physics Letters, 2006, 420, 60-64.	2.6	25
133	Octahedrality versus tetrahedrality in stoichiometric ceria nanoparticles. Chemical Communications, 2012, 48, 4199.	4.1	25
134	Energetic Stability of Absorbed H in Pd and Pt Nanoparticles in a More Realistic Environment. Journal of Physical Chemistry C, 2015, 119, 5180-5186.	3.1	25
135	Adsorption complexes on oxides: Density functional model cluster studies. Theoretical and Computational Chemistry, 1996, , 569-619.	0.4	24
136	Transition metal clusters and supported species with metalâ€“carbon bonds from first-principles quantum chemistry. Journal of Organometallic Chemistry, 2004, 689, 4384-4394.	1.8	24
137	Câ€“O bond scission of methoxide on Pd nanoparticles: A density functional study. Physical Chemistry Chemical Physics, 2006, 8, 2396-2401.	2.8	24
138	Revealing chemical ordering in Ptâ€“Co nanoparticles using electronic structure calculations and X-ray photoelectron spectroscopy. Physical Chemistry Chemical Physics, 2015, 17, 28298-28310.	2.8	24
139	Pt/CeO2 and Pt/CeSnOx Catalysts for Low-Temperature CO Oxidation Prepared by Plasma-Arc Technique. Frontiers in Chemistry, 2019, 7, 114.	3.6	24
140	Density Functional Study of Methane Interaction with Alkali and Alkaline-Earth Metal Cations in Zeolites. Langmuir, 1998, 14, 5559-5567.	3.5	23
141	DFT studies of oxygen dissociation on the 116-atom platinum truncated octahedron particle. Physical Chemistry Chemical Physics, 2014, 16, 26539-26545.	2.8	23
142	Structural and vibrational properties of Ni(111)/NO adsorption complexes: a LCGTO-LDF model cluster investigation. Surface Science, 1994, 307-309, 1193-1199.	1.9	22
143	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.	3.3	22
144	On the electronic and geometric structure of bimetallic clusters. A comparison of the novel cluster Na6Pb to Na6Mg. Chemical Physics Letters, 1995, 245, 671-678.	2.6	20

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145	Reduced ceria nanofilms from structure prediction. Nanoscale, 2015, 7, 4361-4366.	5.6	20
146	Density functional embedded cluster calculations on Lewis acid centers of the Î±-Al2O3(0001) surface: Adsorption of a CO probe. International Journal of Quantum Chemistry, 2002, 90, 386-402.	2.0	19
147	Negatively charged Î¼3-ON species on Ag(111): a LCGTO-LDF cluster analysis of HREELS data. Surface Science, 1993, 287-288, 64-68.	1.9	18
148	Destabilization of adsorbed CO on the Pd(111) surface by subsurface carbon: Density functional studies. Chemical Physics Letters, 2006, 432, 184-189.	2.6	18
149	Hydrogen-bonding effects on electronicg-tensors of semiquinone anion radicals: Relativistic density functional investigation. International Journal of Quantum Chemistry, 2002, 90, 1404-1413.	2.0	17
150	Electronic g values of Na+â€“NO and Cu+â€“NO complexes in zeolites: Analysis using a relativistic density functional method. Physical Chemistry Chemical Physics, 2003, 5, 2429-2434.	2.8	16
151	Unraveling the Surface Chemistry and Structure in Highly Active Sputtered Pt₃Y Catalyst Films for the Oxygen Reduction Reaction. ACS Applied Materials & Interfaces, 2020, 12, 4454-4462.	8.0	16
152	Bonding and vibrations of CHxO and CHx species (x=1â€“3) on a palladium nanoparticle representing model catalysts. Chemical Physics Letters, 2011, 506, 92-97.	2.6	15
153	Structural transformations and adsorption properties of PtNi nanoalloy thin film electrocatalysts prepared by magnetron co-sputtering. Electrochimica Acta, 2017, 251, 427-441.	5.2	15
154	AgPd, AuPd, and AuPt Nanoalloys with Ag- or Au-Rich Compositions: Modeling Chemical Ordering and Optical Properties. Journal of Physical Chemistry C, 2021, 125, 17372-17384.	3.1	15
155	Tungsten Atoms and Clusters Adsorbed on the MgO(001) Surface:Â A Density Functional Study. Journal of Physical Chemistry B, 2000, 104, 11506-11514.	2.6	14
156	On the adsorption and formation of Pt dimers on the CeO2(111) surface. Journal of Chemical Physics, 2011, 135, 244708.	3.0	14
157	Electronâ€Deficient Palladium Clusters in Zeolites and Their Complexes with Probe CO Molecules. A Density Functional Model Cluster Study. Zeitschrift Fur Elektrotechnik Und Elektrochemie, 1996, 100, 413-417.	0.9	12
158	Structure and vibrations of adsorption complexes NH3Ru(001): Density functional model cluster studies. Journal of Molecular Catalysis A, 1997, 119, 245-251.	4.8	12
159	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.	5.4	12
160	Quantifying interactions on interfaces between metal particles and oxide supports in catalytic nanomaterials. NPG Asia Materials, 2022, 14, .	7.9	12
161	Redox-mediated conversion of atomically dispersed platinum to sub-nanometer particles. Journal of Materials Chemistry A, 2017, 5, 9250-9261.	10.3	11
162	Atomic Ordering and Sn Segregation in Ptâ€“Sn Nanoalloys Supported on CeO2 Thin Films. Topics in Catalysis, 2017, 60, 522-532.	2.8	11

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