Gianfranco Pacchioni

List of Publications by Year
in descending order

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596 papers	36,706 citations	2797 94 h-index	5820 161 g-index
638 all docs	638 docs citations	638 times ranked	22807 citing authors

#	Article	IF	Citations
1	Characterization of Paramagnetic Species in N-Doped TiO2 Powders by EPR Spectroscopy and DFT Calculations. Journal of Physical Chemistry B, 2005, 109, 11414-11419.	1.2	928
2	N-doped TiO2: Theory and experiment. Chemical Physics, 2007, 339, 44-56.	0.9	864
3	Origin of Photoactivity of Nitrogen-Doped Titanium Dioxide under Visible Light. Journal of the American Chemical Society, 2006, 128, 15666-15671.	6.6	818
4	Theory of Carbon Doping of Titanium Dioxide. Chemistry of Materials, 2005, 17, 6656-6665.	3.2	663
5	Reduced and n-Type Doped TiO₂: Nature of Ti³⁺ Species. Journal of Physical Chemistry C, 2009, 113, 20543-20552.	1.5	652
6	Electronic Structure of Defect States in Hydroxylated and Reduced RutileTiO2(110)Surfaces. Physical Review Letters, 2006, 97, 166803.	2.9	592
7	Increasing Oxide Reducibility: The Role of Metal/Oxide Interfaces in the Formation of Oxygen Vacancies. ACS Catalysis, 2017, 7, 6493-6513.	5.5	589
8	Origin of the different photoactivity ofN-doped anatase and rutileTiO2. Physical Review B, 2004, 70, .	1.1	508
9	Oxide ultra-thin films on metals: new materials for the design of supported metal catalysts. Chemical Society Reviews, 2008, 37, 2224.	18.7	500
10	Excess electron states in reduced bulk anatase TiO2: Comparison of standard GGA, GGA+U, and hybrid DFT calculations. Journal of Chemical Physics, 2008, 129, 154113.	1.2	472
11	Oxygen Vacancy: The Invisible Agent on Oxide Surfaces. ChemPhysChem, 2003, 4, 1041-1047.	1.0	424
12	Acetylene Cyclotrimerization on Supported Size-Selected Pdn Clusters (1 â‰¤ n â‰¤ 30): One Atom Is Enough!. Journal of the American Chemical Society, 2000, 122, 3453-3457.	6.6	410
13	Structural evolution of atomically dispersed Pt catalysts dictates reactivity. Nature Materials, 2019, 18, 746-751.	13.3	404
14	Charging of Metal Atoms on UltrathinMgO/Mo(100)Films. Physical Review Letters, 2005, 94, 226104.	2.9	338
15	The Nature of Defects in Fluorine-Doped TiO₂. Journal of Physical Chemistry C, 2008, 112, 8951-8956.	1.5	330
16	Control of the Charge State of Metal Atoms on Thin MgO Films. Physical Review Letters, 2007, 98, 096107.	2.9	310
17	Ab Initio Cluster Model Calculations on the Chemisorption of CO2 and SO2 Probe Molecules on MgO and CaO (100) Surfaces. A Theoretical Measure of Oxide Basicity. Journal of the American Chemical Society, 1994, 116, 10152-10158.	6.6	301
18	Trends in non-metal doping of anatase TiO2: B, C, N and F. Catalysis Today, 2013, 206, 12-18.	2.2	284

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19	Mechanisms responsible for chemical shifts of core-level binding energies and their relationship to chemical bonding. Journal of Electron Spectroscopy and Related Phenomena, 1999, 100, 215-236.	0.8	280
20	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.	1.2	272
21	Bonding Trends and Dimensionality Crossover of Gold Nanoclusters on Metal-Supported MgO Thin Films. Physical Review Letters, 2006, 97, 036106.	2.9	268
22	Electron Transfer at Oxide Surfaces. The MgO Paradigm: from Defects to Ultrathin Films. Chemical Reviews, 2013, 113, 4035-4072.	23.0	265
23	Electronic and Structural Properties of WO₃: A Systematic Hybrid DFT Study. Journal of Physical Chemistry C, 2011, 115, 8345-8353.	1.5	250
24	Theoretical description of hole localization in a quartz Al center: The importance of exact electron exchange. Physical Review B, 2000, 63, .	1.1	241
25	Doping of WO₃ for Photocatalytic Water Splitting: Hints from Density Functional Theory. Journal of Physical Chemistry C, 2012, 116, 8901-8909.	1.5	241
26	Electronic Structure of F and V Centers on the MgO Surface. The Journal of Physical Chemistry, 1995, 99, 17010-17018.	2.9	231
27	Tuning the surface metal work function by deposition of ultrathin oxide films: Density functional calculations. Physical Review B, 2006, 73, .	1.1	231
28	Molecular orbital cluster model study of bonding and vibrations of CO adsorbed on MgO surface. International Journal of Quantum Chemistry, 1992, 42, 1115-1139.	1.0	223
29	Modeling doped and defective oxides in catalysis with density functional theory methods: Room for improvements. Journal of Chemical Physics, 2008, 128, 182505.	1.2	221
30	Electronic interactions and charge transfers of metal atoms and clusters on oxide surfaces. Physical Chemistry Chemical Physics, 2013, 15, 1737.	1.3	203
31	Silicon and germanium clusters. A theoretical study of their electronic structures and properties. Journal of Chemical Physics, 1986, 84, 3301-3310.	1.2	194
32	The Interplay between Structure and CO Oxidation Catalysis on Metalâ€Supported Ultrathin Oxide Films. Angewandte Chemie - International Edition, 2010, 49, 4418-4421.	7.2	191
33	Ab initiotheory of optical transitions of point defects inSiO2. Physical Review B, 1998, 57, 818-832.	1.1	189
34	Density Functional Theory and Electron Paramagnetic Resonance Study on the Effect of Nâ^'F Codoping of TiO₂. Chemistry of Materials, 2008, 20, 3706-3714.	3.2	189
35	Nature of stable single atom Pt catalysts dispersed on anatase TiO2. Journal of Catalysis, 2018, 367, 104-114.	3.1	189
36	Quenching of Magnetic Moments by Ligand-Metal Interactions in Nanosized Magnetic Metal Clusters. Physical Review Letters, 1994, 73, 1432-1435.	2.9	181

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37	Characterization of oxide surfaces by infrared spectroscopy of adsorbed carbon monoxide: a theoretical investigation of the frequency shift of CO on MgO and NiO. Surface Science, 1991, 255, 344-354.	0.8	180
38	Work function changes induced by deposition of ultrathin dielectric films on metals: A theoretical analysis. Physical Review B, 2008, 78, .	1.1	180
39	Metal Deposition on Oxide Surfaces:Â A Quantum-Chemical Study of the Interaction of Rb, Pd, and Ag Atoms with the Surface Vacancies of MgO. The Journal of Physical Chemistry, 1996, 100, 9032-9037.	2.9	172
40	QUANTUM CHEMISTRY OF OXIDE SURFACES: FROM CO CHEMISORPTION TO THE IDENTIFICATION OF THE STRUCTURE AND NATURE OF POINT DEFECTS ON MgO. Surface Review and Letters, 2000, 07, 277-306.	0.5	170
41	Supported nickel and copper clusters on MgO(100): A firstâ€principles calculation on the metal/oxide interface. Journal of Chemical Physics, 1996, 104, 7329-7337.	1.2	167
42	Boron-Doped Anatase TiO₂: Pure and Hybrid DFT Calculations. Journal of Physical Chemistry C, 2009, 113, 220-228.	1.5	165
43	Charge density topological study of bonding in lithium clusters. Theoretica Chimica Acta, 1987, 72, 433-458.	0.9	157
44	Oxide Films at the Nanoscale: New Structures, New Functions, and New Materials. Accounts of Chemical Research, 2011, 44, 1244-1252.	7.6	156
45	Controlling the charge state of supported nanoparticles in catalysis: lessons from model systems. Chemical Society Reviews, 2018, 47, 8474-8502.	18.7	155
46	Interaction of Gold Clusters with Color Centers on MgO(001) Films. Angewandte Chemie - International Edition, 2006, 45, 2630-2632.	7.2	154
47	Au Atoms and Dimers on the MgO(100) Surface:Â A DFT Study of Nucleation at Defects. Journal of Physical Chemistry B, 2005, 109, 8040-8048.	1.2	149
48	Nature of Ti Interstitials in Reduced Bulk Anatase and Rutile TiO₂. Journal of Physical Chemistry C, 2009, 113, 3382-3385.	1.5	148
49	Paramagnetic Defects in Polycrystalline Zirconia: An EPR and DFT Study. Chemistry of Materials, 2013, 25, 2243-2253.	3.2	148
50	Physisorbed and chemisorbed CO2 at surface and step sites of the MgO(100) surface. Surface Science, 1993, 281, 207-219.	0.8	146
51	Electronic properties of rutileTiO2ultrathin films: Odd-even oscillations with the number of layers. Physical Review B, 2004, 70, .	1.1	144
52	Excess Electrons Stabilized on Ionic Oxide Surfacesâ€. Accounts of Chemical Research, 2006, 39, 861-867.	7.6	144
53	Identification of Color Centers on MgO(001) Thin Films with Scanning Tunneling Microscopy. Journal of Physical Chemistry B, 2006, 110, 46-49.	1.2	143
54	Adhesion energy of Cu atoms on the MgO(001) surface. Journal of Chemical Physics, 1999, 110, 4873-4879.	1.2	140

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55	Electronic structure and phase stability of oxide semiconductors: Performance of dielectric-dependent hybrid functional DFT, benchmarked against<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:mrow><mml:mi>G</mml:mi><mml:mi>W</mml:mi></mml:mrow></mml:math> structure calculations and experiments. Physical Review B, 2015, 91, .	1.1	140
56	Studies of the Cuî—¸O bond in cupric oxide by X-ray photoelectron spectroscopy and ab initio electronic structure models. Journal of Electron Spectroscopy and Related Phenomena, 1992, 59, 255-269.	0.8	138
57	Computed Optical Absorption and Photoluminescence Spectra of Neutral Oxygen Vacancies inÎ±-Quartz. Physical Review Letters, 1997, 79, 753-756.	2.9	138
58	Semiconductor-to-metal transition in WO<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:msub><mml:mrow /><mml:mrow><mml:mn>3</mml:mn><mml:mo>â^'</mml:mo><mml:mi>x</mml:mi></mml:mrow></mml:msub></mml:math>: Nature of the oxygen vacancy. Physical Review B, 2011, 84, .	1.1	136
59	Hydrogen Adsorption and Diffusion on the Anatase TiO₂(101) Surface: A First-Principles Investigation. Journal of Physical Chemistry C, 2011, 115, 6809-6814.	1.5	136
60	First Principles Study of Nitrogen Doping at the Anatase TiO2(101) Surface. Journal of Physical Chemistry C, 2007, 111, 9275-9282.	1.5	135
61	Paramagnetic Defect Centers at the MgO Surface. An Alternative Model to Oxygen Vacancies. Journal of the American Chemical Society, 2003, 125, 738-747.	6.6	134
62	Rational Band Gap Engineering of WO₃ Photocatalyst for Visible light Water Splitting. ChemCatChem, 2012, 4, 476-478.	1.8	134
63	Structure and stability of oxygen vacancies on sub-surface, terraces, and low-coordinated surface sites of MgO:. Surface Science, 1998, 412-413, 657-671.	0.8	132
64	Ketonization of Carboxylic Acids in Biomass Conversion over TiO₂ and ZrO₂ Surfaces: A DFT Perspective. ACS Catalysis, 2014, 4, 2874-2888.	5.5	132
65	A Combined EPR and Quantum Chemical Approach to the Structure of Surface Fs+(H) Centers on MgO. Journal of Physical Chemistry B, 1997, 101, 971-982.	1.2	131
66	Cu, Ag, and Au atoms adsorbed on TiO2(110): cluster and periodic calculations. Surface Science, 2001, 471, 21-31.	0.8	131
67	Metal-phosphine bonding revisited. .sigma.-Basicity, .pi.-acidity, and the role of phosphorus d orbitals in zerovalent metal-phospine complexes. Inorganic Chemistry, 1992, 31, 4391-4398.	1.9	129
68	Interplay between structural, magnetic, and electronic properties in a<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:mi mathvariant="normal">Fe</mml:mi><mml:mi mathvariant="normal">O</mml:mi><mml:mo>â^•</mml:mo><mml:mi mathvariant="normal">Pt</mml:mi><mml:mrow><mml:mo>(</mml:mo><mml:mn>111</mml:mn><mml:mo>)</mml:mo></mml:mrow></mml:math> film. Physical Review B, 2007, 76, .	1.1	129
69	Bond ionicity of the halogenâ€“silver interaction. Journal of Chemical Physics, 1989, 90, 4287-4295.	1.2	126
70	Charging of Au Atoms on TiO2Thin Films from CO Vibrational Spectroscopy and DFT Calculations. Journal of Physical Chemistry B, 2005, 109, 18418-18426.	1.2	126
71	Cluster and band structure ab initio calculations on the adsorption of CO on acid sites of the TiO2(110) surface. Surface Science, 1996, 350, 159-175.	0.8	125
72	Photoluminescence of atomic gold and silver particles in soda-lime silicate glasses. Nanotechnology, 2008, 19, 135701.	1.3	122

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73	Hydrogen Adsorption, Dissociation, and Spillover on Ru₁₀ Clusters Supported on Anatase TiO₂ and Tetragonal ZrO₂ (101) Surfaces. ACS Catalysis, 2015, 5, 5486-5495.	5.5	122
74	Ab initio theory of point defects in oxide materials: structure, properties, chemical reactivity. Solid State Sciences, 2000, 2, 161-179.	1.5	121
75	Binding of Single Gold Atoms on Thin MgO(001) Films. Physical Review Letters, 2006, 96, 146804.	2.9	120
76	Spectroscopic Properties of Doped and Defective Semiconducting Oxides from Hybrid Density Functional Calculations. Accounts of Chemical Research, 2014, 47, 3233-3241.	7.6	119
77	Electronic structure of a neutral oxygen vacancy inSrTiO3. Physical Review B, 2003, 68, .	1.1	116
78	Optical Absorption and Nonradiative Decay Mechanism ofEâ€²Center in Silica. Physical Review Letters, 1998, 81, 377-380.	2.9	113
79	Electronic structure of an isolated oxygen vacancy at the TiO2(110) surface. Chemical Physics Letters, 2002, 355, 417-423.	1.2	112
80	Chemisorption of CO on defect sites of MgO. Surface Science, 1992, 275, 450-458.	0.8	111
81	Charging of Metal Adatoms on Ultrathin Oxide Films: Au and Pd on<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mi>FeO</mml:mi><mml:mo>/</mml:mo><mml:mi>Pt</mml:mi><mml:mo stretchy="false">(</mml:mo><mml:mn>111</mml:mn><mml:mo) Tj ETQq1 1 0.784314 rgBT /Overlock 10 Tf 50 407 Td (stretchy="fa	2.9	109
82	Characteristics ofPdadsorption on theMgO(100)surface: Role of oxygen vacancies. Physical Review B, 2001, 64, .	1.1	108
83	Identification of Defect Sites on MgO(100) Thin Films by Decoration with Pd Atoms and Studying CO Adsorption Properties. Journal of the American Chemical Society, 2001, 123, 6172-6178.	6.6	108
84	Ab initioformation energies of point defects in pure and Ge-dopedSiO2. Physical Review B, 1997, 56, 7304-7312.	1.1	107
85	Formation of Superoxide Anions on Ceria Nanoparticles by Interaction of Molecular Oxygen with Ce³⁺ Sites. Journal of Physical Chemistry C, 2011, 115, 5817-5822.	1.5	107
86	Transition levels of defect centers in ZnO by hybrid functionals and localized basis set approach. Journal of Chemical Physics, 2010, 133, 144512.	1.2	106
87	Measures of ionicity of alkaline-earth oxides from the analysis ofab initiocluster wave functions. Physical Review B, 1993, 48, 11573-11582.	1.1	105
88	CO Oxidation on a Au/TiO₂ Nanoparticle Catalyst via the Au-Assisted Marsâ€“van Krevelen Mechanism. ACS Catalysis, 2018, 8, 6513-6525.	5.5	103
89	Nucleation of Pd Dimers at Defect Sites of the MgO(100) Surface. Physical Review Letters, 2004, 92, 096105.	2.9	101
90	When the Reporter Induces the Effect: Unusual IR spectra of CO on Au1/MgO(001)/Mo(001). Angewandte Chemie - International Edition, 2006, 45, 2633-2635.	7.2	101

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91	Activation of Oxygen on MgO: O₂^{â˜} Radical Ion Formation on Thin, Metalâ€Supported MgO(001) Films. Angewandte Chemie - International Edition, 2011, 50, 2635-2638.	7.2	101
92	A theoretical study of the adsorption and reaction of SO2 at surface and step sites of the MgO(100) surface. Surface Science, 1994, 315, 337-350.	0.8	99
93	Tailoring the Shape of Metal Adâ€Particles by Doping the Oxide Support. Angewandte Chemie - International Edition, 2011, 50, 11525-11527.	7.2	99
94	Relativistic effects in the electronic structure of the monoxides and monocarbonyls of Ni, Pd, and Pt: Local and gradientâ€corrected density functional calculations. Journal of Chemical Physics, 1995, 102, 3695-3702.	1.2	96
95	Cluster and periodic ab-initio calculations on K/TiO2(110). Surface Science, 1998, 418, 150-165.	0.8	95
96	Colour centres at the surface of alkali-earth oxides. A new hypothesis on the location of surface electron traps. Surface Science, 1999, 421, 246-262.	0.8	95
97	Measuring the Charge State of Point Defects on MgO/Ag(001). Journal of the American Chemical Society, 2009, 131, 17544-17545.	6.6	95
98	Adsorption of Cu, Pd, and Cs Atoms on Regular and Defect Sites of the SiO2Surface. Journal of the American Chemical Society, 1999, 121, 813-821.	6.6	94
99	Cationic and anionic vacancies on the NiO(100) surface: DFT+U and hybrid functional density functional theory calculations. Journal of Chemical Physics, 2007, 127, 174711.	1.2	93
100	Nature of Ag Islands and Nanoparticles on the CeO₂(111) Surface. Journal of Physical Chemistry C, 2012, 116, 1122-1132.	1.5	92
101	Optical transitions and EPR properties of two-coordinated Si, Ge, Sn and relatedH(I),H(II),andH(III)centers in pure and doped silica fromab initiocalculations. Physical Review B, 1998, 58, 6090-6096.	1.1	91
102	Oxygen-Induced Transformations of an FeO(111) Film on Pt(111): A Combined DFT and STM Study. Journal of Physical Chemistry C, 2010, 114, 21504-21509.	1.5	90
103	Donor Characteristics of Transition-Metal-Doped Oxides: Cr-Doped MgO versus Mo-Doped CaO. Journal of the American Chemical Society, 2012, 134, 11380-11383.	6.6	90
104	Adsorption of Pd atoms and Pd4 clusters on the MgO(001) surface: a density functional study. Chemical Physics Letters, 1997, 275, 245-252.	1.2	88
105	Theoretical analysis of the vibrational shifts of CO chemisorbed on Pd(100). Surface Science, 1990, 236, 233-240.	0.8	87
106	Cr/Sb co-doped TiO2 from first principles calculations. Chemical Physics Letters, 2009, 469, 166-171.	1.2	87
107	The nitrogen photoactive centre in N-doped titanium dioxide formed via interaction of N atoms with the solid. Nature and energy level of the species. Chemical Physics Letters, 2009, 477, 135-138.	1.2	87
108	Cyclization of acetylene over Pd(111): a theoretical study of reaction mechanisms and surface intermediates. Surface Science, 1994, 304, 208-222.	0.8	85

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109	Importance of Madelung potential in quantum chemical modeling of ionic surfaces. Journal of Computational Chemistry, 1997, 18, 617-628.	1.5	85
110	Optical properties of surface and bulk F centers in MgO from ab initio cluster model calculations. Journal of Chemical Physics, 1998, 108, 7835-7841.	1.2	85
111	DFT Study of Hydrogen Adsorption On the Monoclinic WO₃ (001) Surface. Journal of Physical Chemistry C, 2012, 116, 10672-10679.	1.5	85
112	Structure and Properties of Zirconia Nanoparticles from Density Functional Theory Calculations. Journal of Physical Chemistry C, 2016, 120, 4392-4402.	1.5	85
113	Defect calculations in semiconductors through a dielectric-dependent hybrid DFT functional: The case of oxygen vacancies in metal oxides. Journal of Chemical Physics, 2015, 143, 134702.	1.2	84
114	Pd and Ag dimers and tetramers adsorbed at the MgO(001) surface: a density functional study. Physical Chemistry Chemical Physics, 1999, 1, 4655-4661.	1.3	83
115	Bonding of Pd, Ag, and Au atoms on MgO(100) surfaces andMgOâ•Mo(100)ultra-thin films: A comparative DFT study. Physical Review B, 2005, 72, .	1.1	82
116	Charge transfers at metal/oxide interfaces: a DFT study of formation of KÎ´+and AuÎ´â”species on MgO/Ag(100) ultra-thin films from deposition of neutral atoms. Physical Chemistry Chemical Physics, 2006, 8, 3335-3341.	1.3	82
117	Cluster models of O2â” adsorption on regular and defect sites and Fs centers of the MgO (100) surface. Chemical Physics Letters, 1996, 255, 58-64.	1.2	81
118	Nature of the Chemical Bond between Metal Atoms and Oxide Surfaces:Â New Evidences from Spin Density Studies of K Atoms on Alkaline Earth Oxides. Journal of the American Chemical Society, 2005, 127, 16935-16944.	6.6	81
119	Twoâ€Đimensional Oxides: Multifunctional Materials for Advanced Technologies. Chemistry - A European Journal, 2012, 18, 10144-10158.	1.7	81
120	Optical Absorption Spectrum of Gold Atoms Deposited onSiO2from Cavity Ringdown Spectroscopy. Physical Review Letters, 2005, 94, 213402.	2.9	80
121	H₂O Adsorption on WO₃ and WO_{3â€“x} (001) Surfaces. ACS Applied Materials & Interfaces, 2017, 9, 23212-23221.	4.0	79
122	Adsorption of Ruthenium Atoms and Clusters on Anatase TiO₂ and Tetragonal ZrO₂(101) Surfaces: A Comparative DFT Study. Journal of Physical Chemistry C, 2015, 119, 10856-10868.	1.5	78
123	Calculated properties of alkali metal clusters with fivefold symmetry. Journal of Chemical Physics, 1984, 80, 325-328.	1.2	77
124	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.	1.2	77
125	Role of Dihydride and Dihydrogen Complexes in Hydrogen Evolution Reaction on Single-Atom Catalysts. Journal of the American Chemical Society, 2021, 143, 20431-20441.	6.6	77
126	Electronic Structure and Properties of Small Al and Ge Clusters. Zeitschrift Fur Elektrotechnik Und Elektrochemie, 1984, 88, 242-245.	0.9	76

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127	Quantum-Chemical Study of Electrochemical Promotion in Catalysis. The Journal of Physical Chemistry, 1996, 100, 16653-16661.	2.9	76
128	The contribution of metal sp electrons to the chemisorption of CO: theoretical studies of CO on Li, Na, and Cu. Surface Science, 1992, 278, 427-436.	0.8	75
129	Measure of Surface Potential at the Aqueousâ€“Oxide Nanoparticle Interface by XPS from a Liquid Microjet. Nano Letters, 2013, 13, 5403-5407.	4.5	75
130	Single Electron Traps at the Surface of Polycrystalline MgO:Â Assignment of the Main Trapping Sites. Journal of Physical Chemistry B, 2005, 109, 7314-7322.	1.2	74
131	Tungsten Oxide in Catalysis and Photocatalysis: Hints from DFT. Topics in Catalysis, 2013, 56, 1404-1419.	1.3	74
132	A DFT study of the acidâ€“base properties of anatase TiO2 and tetragonal ZrO2 by adsorption of CO and CO2 probe molecules. Surface Science, 2016, 652, 163-171.	0.8	74
133	Comparative study of tetramers built from Ia, IIa, IIIa, and IVa atoms. Surface Science, 1985, 156, 650-669.	0.8	73
134	Optical properties of point defects in SiO2 from time-dependent density functional theory. Journal of Chemical Physics, 2002, 116, 825-831.	1.2	73
135	Five-coordination in platinum(II) species: when and why. Journal of the Chemical Society Chemical Communications, 1992, , 333.	2.0	72
136	Cerium-Doped Zirconium Dioxide, a Visible-Light-Sensitive Photoactive Material of Third Generation. Journal of Physical Chemistry Letters, 2014, 5, 447-451.	2.1	71
137	Gold and Silver Clusters on TiO₂ and ZrO₂ (101) Surfaces: Role of Dispersion Forces. Journal of Physical Chemistry C, 2015, 119, 15381-15389.	1.5	70
138	Anisotropic Effects of Oxygen Vacancies on Electrochromic Properties and Conductivity of Î³-Monoclinic WO₃. Journal of Physical Chemistry C, 2016, 120, 11716-11726.	1.5	70
139	Chemical Bonding and Electronic Structure of Small Homonuclear Clusters of Elements of Groups IA, IIA, IIIA and IVA. Zeitschrift Fur Elektrotechnik Und Elektrochemie, 1983, 87, 503-512.	0.9	69
140	Ab initio MRD CI investigation of the optical spectra of C4 and C5 clusters. Journal of Chemical Physics, 1988, 88, 1066-1073.	1.2	69
141	Carbonylated Nickel Clusters: From Molecules to Metals. Accounts of Chemical Research, 1995, 28, 390-397.	7.6	69
142	H2Cracking at SiO2Defect Centersâ€. Journal of Physical Chemistry A, 2000, 104, 4674-4684.	1.1	69
143	Reductive Activation of the Nitrogen Molecule at the Surface of â€œElectron-Richâ€•MgO and CaO. The N2-Surface Adsorbed Radical Ion. Journal of Physical Chemistry B, 2001, 105, 497-505.	1.2	69
144	First Evidence of a Single-Ion Electron Trap at the Surface of an Ionic Oxide. Angewandte Chemie - International Edition, 2003, 42, 1759-1761.	7.2	69

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145	Alkali adsorbates on metal surfaces: observable consequences of the ionic K/Cu(100) interaction. Surface Science, 1993, 286, 317-326.	0.8	68
146	Electronic structure ofNiOâˆ•Ag(100)thin films fromDFT+Uand hybrid functional DFT approaches. Physical Review B, 2006, 74, .	1.1	68
147	Azide-Alkyne Click Chemistry over a Heterogeneous Copper-Based Single-Atom Catalyst. ACS Catalysis, 2022, 12, 2947-2958.	5.5	68
148	Point-charge effects on the vibrational frequency of CO chemisorbed on Cu and Pd clusters: A model for CO with ionic coadsorbates. Physical Review B, 1989, 40, 6003-6011.	1.1	67
149	Mechanisms responsible for the shifts of core-level binding energies between surface and bulk atoms of metals. Surface Science Reports, 1993, 19, 265-283.	3.8	67
150	Cluster calculations of CO chemisorbed on the bridge site of Pd(100). Journal of Chemical Physics, 1990, 93, 1209-1214.	1.2	66
151	Structure and vibrational spectra of crystalline SiO2 ultra-thin films on Mo(112). Surface Science, 2005, 584, 225-236.	0.8	65
152	Ab initio study of the optical transitions of F centers at low-coordinated sites of the MgO surface. Surface Science, 1999, 429, 217-228.	0.8	64
153	Charge-induced formation of linear Au clusters on thin MgO films: Scanning tunneling microscopy and density-functional theory study. Physical Review B, 2008, 78, .	1.1	64
154	Is CO chemisorbed on Pt anomalous compared with Ni and Pd? An example of surface chemistry dominated by relativistic effects. Surface Science, 1997, 392, 173-184.	0.8	63
155	Electron trapping at neutral divacancy sites on the MgO surface. Journal of Chemical Physics, 2002, 117, 2844-2851.	1.2	63
156	Effect of Alkali Metals Interstitial Doping on Structural and Electronic Properties of WO₃. Journal of Physical Chemistry C, 2014, 118, 3000-3006.	1.5	63
157	Can corundum be described as an ionic oxide?. Journal of Chemical Physics, 1993, 99, 6818-6823.	1.2	62
158	Au Dimers on Thin MgO(001) Films: Flat and Charged or Upright and Neutral?. Journal of the American Chemical Society, 2008, 130, 7814-7815.	6.6	62
159	Coordination modes of histidine. 3. Stereochemistry of copper(II) complexes related to pyridoxal catalysis. Journal of the American Chemical Society, 1982, 104, 2386-2396.	6.6	61
160	On the evolution of cluster to bulk properties: a theoretical LCGTO-LDF study of free and coordinated Nin clusters (n=6-147). Chemical Physics, 1994, 184, 125-137.	0.9	61
161	Formation of oxygen active species in Ag-modified CeO2 catalyst for soot oxidation: A DFT study. Catalysis Today, 2011, 177, 31-38.	2.2	61
162	Theoretical study of the interaction of carbon monoxide with palladium clusters: relations between surface and organometallic chemistry. The Journal of Physical Chemistry, 1987, 91, 2658-2664.	2.9	60

#	Article	IF	Citations
163	Final state effects for the core-level XPS spectra of NiO. Chemical Physics Letters, 1993, 207, 569-574.	1.2	60
164	Origin of Visible Light Photoactivity of the CeO₂/ZnO Heterojunction. ACS Applied Energy Materials, 2018, 1, 4247-4260.	2.5	60
165	Universal Principles for the Rational Design of Single Atom Electrocatalysts? Handle with Care. ACS Catalysis, 2022, 12, 5846-5856.	5.5	60
166	Cluster model calculations of oxygen vacancies in SiO2and MgO Formation energies, optical transitions and EPR spectra. Faraday Discussions, 1997, 106, 155-172.	1.6	59
167	Chemisorption and Reactivity of Methanol on MgO Thin Films. Journal of Physical Chemistry B, 2002, 106, 11961-11969.	1.2	59
168	Accuracy of dielectric-dependent hybrid functionals in the prediction of optoelectronic properties of metal oxide semiconductors: a comprehensive comparison with many-bodyGWand experiments. Journal of Physics Condensed Matter, 2018, 30, 044003.	0.7	59
169	Electric field effects on the surfaceâ€"adsorbate interaction: cluster model studies. Electrochimica Acta, 1991, 36, 1669-1675.	2.6	58
170	CO adsorption on SnO2(110): cluster and periodic ab initio calculations. Surface Science, 2000, 461, 54-66.	0.8	58
171	Band gap engineering of bulk ZrO2 by Ti doping. Physical Chemistry Chemical Physics, 2011, 13, 17667.	1.3	58
172	Electric field effects in heterogeneous catalysis. Journal of Molecular Catalysis A, 1997, 119, 263-273.	4.8	57
173	A quantum-chemical study of Pd atoms and dimers supported on TiO2(110) and their interaction with CO. Surface Science, 1999, 426, 106-122.	0.8	57
174	Properties of MgO(100) ultrathin layers on Pd(100):â€ƒInfluence of the metal support. Physical Review B, 2003, 67, .	1.1	57
175	From Heterolytic to Homolytic H₂ Dissociation on Nanostructured MgO(001) Films As a Function of the Metal Support. Journal of Physical Chemistry C, 2013, 117, 10623-10629.	1.5	57
176	Molecular orbital theory for the analysis of photoemission spectra. Journal of Electron Spectroscopy and Related Phenomena, 1990, 51, 69-74.	0.8	55
177	Ionicity of K chemisorbed on a Cu surface. Surface Science, 1992, 269-270, 669-676.	0.8	55
178	Modeling of supported metal clusters: a density functional study of CO chemisorption on Ni clusters deposited on alumina. Surface Science, 1994, 306, 169-178.	0.8	55
179	Surface reactivity of MgO oxygen vacancies: electrostatic mechanisms in the formation of O2â˜' and COâ˜' species. Journal of Chemical Physics, 1997, 107, 2066-2078.	1.2	55
180	Investigation of alkali-metal clusters with pseudopotential multireference double-excitation configuration interaction method. Chemical Physics Letters, 1982, 87, 151-158.	1.2	54

#	Article	IF	Citations
181	EPR and IR spectral properties of hydrogen-associated bulk and surface defects inSiO2:Ab initiocalculations. Physical Review B, 1998, 58, 7745-7752.	1.1	54
182	CO Oxidation on Au Nanoparticles Supported on ZrO₂: Role of Metal/Oxide Interface and Oxide Reducibility. ChemCatChem, 2017, 9, 1119-1127.	1.8	54
183	Chemical shifts of the core-level binding energies for the alkaline-earth oxides. Chemical Physics Letters, 1992, 196, 641-646.	1.2	53
184	Acetylene on Cu and Pd(111) surfaces: a comparative theoretical study of bonding mechanism, adsorption sites, and vibrational spectra. Surface Science, 1996, 346, 91-107.	0.8	53
185	Surface core-level spectroscopy of Cu(100) and Al(100). Physical Review B, 1991, 43, 5172-5175.	1.1	51
186	The competition between chemical bonding and magnetism in the adsorption of atomic Ni on MgO(100). Journal of Chemical Physics, 2001, 115, 8172-8177.	1.2	50
187	NO Monomers on MgO Powders and Thin Films. Journal of Physical Chemistry B, 2002, 106, 1637-1645.	1.2	50
188	O2 adsorption and dissociation on neutral, positively and negatively charged Aun (n = 5â€“79) clusters. Physical Chemistry Chemical Physics, 2010, 12, 10723.	1.3	50
189	The nitrogenâ€“boron paramagnetic center in visible light sensitized Nâ€“B co-doped TiO₂. Experimental and theoretical characterization. Physical Chemistry Chemical Physics, 2011, 13, 136-143.	1.3	50
190	Al- and Ga-Doped TiO₂, ZrO₂, and HfO₂: The Nature of O 2p Trapped Holes from a Combined Electron Paramagnetic Resonance (EPR) and Density Functional Theory (DFT) Study. Chemistry of Materials, 2015, 27, 3936-3945.	3.2	50
191	Interfacing single-atom catalysis with continuous-flow organic electrosynthesis. Chemical Society Reviews, 2022, 51, 3898-3925.	18.7	50
192	Structure and stability of lithium (Li4 and Li6) clusters. The Journal of Physical Chemistry, 1983, 87, 1096-1097.	2.9	49
193	Ïƒâ”Ï€ Contributions in metal-co bond: A theoretical study of RhCO and PdCO. Chemical Physics, 1985, 99, 87-101.	0.9	49
194	New bonding mode of CO on stepped MgO surfaces from density functional cluster model calculations. Chemical Physics Letters, 2000, 320, 345-351.	1.2	49
195	Optical and EPR properties of point defects at a crystalline silica surface:Ab initioembedded-cluster calculations. Physical Review B, 2007, 75, .	1.1	49
196	Adsorption of metal adatoms on FeO(111) and MgO(111) monolayers: Effects of charge state of adsorbate on rumpling of supported oxide film. Physical Review B, 2009, 80, .	1.1	49
197	First Principles Calculations on Oxide-Based Heterogeneous Catalysts and Photocatalysts: Problems and Advances. Catalysis Letters, 2015, 145, 80-94.	1.4	49
198	Role of Surface Defects in the Activation of Supported Metals:â€‰ A Quantum-Chemical Study of Acetylene Cyclotrimerization on Pd1/MgO. Journal of Physical Chemistry B, 2000, 104, 10612-10617.	1.2	48

#	Article	IF	Citations
199	Nitrogen impurity states in polycrystalline ZnO. A combined EPR and theoretical study. Journal of Materials Chemistry, 2010, 20, 689-697.	6.7	48
200	Complexes of platinum(II) with chiral diamines and guanosine. Stereochemical investigation related to the mechanism of the antitumor activity of cis-bis(amine)platinum(II) type complexes. Inorganic Chemistry, 1982, 21, 2006-2014.	1.9	47
201	CO adsorption on Rh, Pd and Ag atoms deposited on the MgO surface: a comparative ab initio study. Surface Science, 2003, 540, 63-75.	0.8	47
202	Gold Atoms and Dimers on Amorphous SiO2:Â Calculation of Optical Properties and Cavity Ringdown Spectroscopy Measurements. Journal of Physical Chemistry B, 2005, 109, 19876-19884.	1.2	47
203	Enhanced CO Oxidation on the Oxide/Metal Interface: From Ultraâ€High Vacuum to Nearâ€Atmospheric Pressures. ChemCatChem, 2015, 7, 2620-2627.	1.8	47
204	Acetic acid ketonization on tetragonal zirconia: Role of surface reduction. Journal of Catalysis, 2016, 344, 465-473.	3.1	47
205	Structural and electronic properties of bulk and ultrathin layers of V2O5 and MoO3. Computational Materials Science, 2019, 163, 230-240.	1.4	47
206	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
207	Size-effects in the acetylene cyclotrimerization on supported size-selected Pdn clusters (1â‰¤nâ‰¤30). Surface Science, 2000, 454-456, 984-989.	0.8	46
208	Photoabsorption of dioxasilyrane and silanone groups at the surface of silica. Journal of Chemical Physics, 2001, 114, 4657.	1.2	46
209	Oxygen vacancies and peroxo groups on regular and low-coordinated sites of MgO, CaO, SrO, and BaO surfaces. Surface Science, 2006, 600, 1147-1154.	0.8	46
210	Adsorption of Au and Pd on Ruthenium-Supported Bilayer Silica. Journal of Physical Chemistry C, 2014, 118, 20959-20969.	1.5	46
211	Nature of Sinteringâ€Resistant, Singleâ€Atom Ru Species Dispersed on Zirconiaâ€Based Catalysts: A DFT and FTIR Study of CO Adsorption. ChemCatChem, 2018, 10, 2634-2645.	1.8	46
212	Role of Heterojunction in Charge Carrier Separation in Coexposed Anatase (001)â€“(101) Surfaces. Journal of Physical Chemistry Letters, 2019, 10, 2372-2377.	2.1	46
213	Quantum confinement in group IIIâ€“V semiconductor 2D nanostructures. Nanoscale, 2020, 12, 17494-17501.	2.8	46
214	The bond nature of alkaline-earth homonuclear metal clusters investigated with pseudopotential CI method. Chemical Physics, 1982, 71, 181-198.	0.9	45
215	Comparative periodic and cluster ab initio study on. Surface Science, 1997, 373, 21-32.	0.8	45
216	Electron Trapping at Point Defects on Hydroxylated Silica Surfaces. Physical Review Letters, 2007, 99, 136801.	2.9	45

#	Article	IF	Citations
217	Charging of Gold Atoms on Doped MgO and CaO: Identifying the Key Parameters by DFT Calculations. Journal of Physical Chemistry C, 2013, 117, 9943-9951.	1.5	45
218	Band Gap of 3D Metal Oxides and Quasi-2D Materials from Hybrid Density Functional Theory: Are Dielectric-Dependent Functionals Superior?. Journal of Chemical Theory and Computation, 2019, 15, 6294-6312.	2.3	45
219	Stability and other properties of Li13clusters. An example of specific characteristics of clusters. Journal of Chemical Physics, 1984, 81, 3588-3593.	1.2	44
220	Ab Initio Theory of Metal Deposition on SiO2. 1. Cun(n= 1â^'5) Clusters on Nonbridging Oxygen Defects. Journal of Physical Chemistry B, 1999, 103, 1712-1718.	1.2	44
221	Tuning the work function of ultrathin oxide films on metals by adsorption of alkali atoms. Journal of Chemical Physics, 2008, 128, 164707.	1.2	44
222	Rational Design of Semiconductor Heterojunctions for Photocatalysis. Chemistry - A European Journal, 2021, 27, 13306-13317.	1.7	44
223	Pseudopotential SCF and CI investigation of the electronic structure of PdH, PdC and PdCO. Chemical Physics Letters, 1982, 92, 486-492.	1.2	43
224	Size and shape dependence of the electrostatic potential in cluster models of the MgO(100) surface. International Journal of Quantum Chemistry, 1996, 58, 241-250.	1.0	43
225	Ab initio calculations of 29Si solid state NMR chemical shifts of silane and silanol groups in silica. Chemical Physics Letters, 2000, 326, 523-529.	1.2	43
226	Density functional theory study of TiO<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:msub><mml:mrow /><mml:mrow><mml:mn>2</mml:mn></mml:mrow></mml:msub></mml:mrow></mml:math>/Ag interfaces and their role in memristor devices. Physical Review B, 2011, 83, .	1.1	43
227	Atomistic Modeling of Corrosion Resistance: A First Principles Study of O₂ Reduction on the Al(111) Surface Covered with a Thin Hydroxylated Alumina Film. Advanced Materials Interfaces, 2014, 1, 1300072.	1.9	43
228	Role of Oxide Reducibility in the Deoxygenation of Phenol on Ruthenium Clusters Supported on the Anatase Titania (1â€‰0â€‰1) Surface. ChemCatChem, 2016, 8, 2492-2499.	1.8	43
229	Electronic structure and properties of nickel clusters: Ni6, Ni8, Ni19, and Ni44. Chemical Physics Letters, 1992, 199, 275-280.	1.2	42
230	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.	0.8	42
231	Selectivity of Surface Defects for the Activation of Supported Metal Atoms:Â Acetylene Cyclotrimerization on Pd1/MgO. Journal of Physical Chemistry B, 2002, 106, 3173-3181.	1.2	42
232	NO and NO2Adsorption on Terrace, Step, and Corner Sites of the BaO Surface from DFT Calculations. Journal of Physical Chemistry B, 2004, 108, 4752-4758.	1.2	42
233	Acetylene trimerization on Ag, Pd and Rh atoms deposited on MgO thin films. Physical Chemistry Chemical Physics, 2005, 7, 955-962.	1.3	42
234	Tuning the charge state of Ag and Au atoms and clusters deposited on oxide surfaces by doping: a DFT study of the adsorption properties of nitrogen- and niobium-doped TiO₂ and ZrO₂. Physical Chemistry Chemical Physics, 2015, 17, 22342-22360.	1.3	42

#	Article	IF	Citations
235	Covalent and ionic contributions to the bonding of atomic and molecular adsorbates on metal surfaces: A cluster model approach. International Journal of Quantum Chemistry, 1990, 38, 675-689.	1.0	41
236	Hybrid quantum-mechanical and molecular mechanics study of Cu atoms deposition on SiO2 surface defects. Chemical Physics Letters, 1998, 294, 611-618.	1.2	41
237	Au and Pd atoms adsorbed on pure and Ti-doped SiO2âˆ•Mo(112) films. Journal of Chemical Physics, 2006, 124, 034701.	1.2	41
238	Electronic structure and magnetic moments of Co4 and Ni4 clusters supported on the MgO(001) surface. Surface Science, 2001, 473, 213-226.	0.8	40
239	Formation of Schottky Defects at the Surface of MgO, TiO2, and SnO2:Â A Comparative Density Functional Theoretical Study. Journal of Physical Chemistry B, 2004, 108, 12858-12864.	1.2	40
240	Pd nanoclusters at the MgO(100) surface. Surface Science, 2005, 575, 197-209.	0.8	40
241	The structure of a stoichiometric TiO2 nanophase on Pt(1 1 1). Surface Science, 2007, 601, 3488-3496.	0.8	40
242	Ab Initio Study of Transition Levels for Intrinsic Defects in Silicon Nitride. Journal of Physical Chemistry C, 2011, 115, 561-569.	1.5	40
243	Density Functional Theory Estimate of Halide Perovskite Band Gap: When Spin Orbit Coupling Helps. Journal of Physical Chemistry C, 2022, 126, 2184-2198.	1.5	40
244	Structure and bonding in Cr(CO)5H2 and Cr(CO)4(H2)2 complexes. Journal of the American Chemical Society, 1990, 112, 80-85.	6.6	39
245	Paramagnetism of high nuclearity metal cluster compounds as derived from local density functional calculations. Journal of Chemical Physics, 1991, 95, 7004-7007.	1.2	39
246	Surface reactivity of MgO oxygen vacancies. Catalysis Today, 1999, 50, 533-540.	2.2	39
247	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.	2.2	39
248	Paramagnetic centers in Ge-doped silica:â€ƒA first-principles study. Physical Review B, 2000, 62, 5452-5460.	1.1	39
249	Modeling disorder in amorphous silica with embedded clusters:â€ƒThe peroxy bridge defect center. Physical Review B, 2001, 64, .	1.1	39
250	Acetylene polymerization on supported transition metal clusters. Journal of Molecular Catalysis A, 2003, 199, 103-113.	4.8	39
251	Formation of CO₂^{â^’} Radical Anions from CO₂ Adsorption on an Electron-Rich MgO Surface: A Combined ab Initio and Pulse EPR Study. Journal of Physical Chemistry C, 2008, 112, 19568-19576.	1.5	39
252	Interaction of Water with FeO(111)/Pt(111): Environmental Effects and Influence of Oxygen. Journal of Physical Chemistry C, 2011, 115, 19328-19335.	1.5	39

#	Article	IF	Citations
253	Bonding of NO to NiO(100) and NixMg1â^'xO(100) surfaces: A challenge for theory. Journal of Chemical Physics, 2002, 117, 2299-2306.	1.2	38
254	Bonding of NH3, CO, and NO to NiO and Ni-doped MgO: a problem for density functional theory. Journal of Physics Condensed Matter, 2004, 16, S2497-S2507.	0.7	38
255	Understanding surface core-level shifts using the Auger parameter: A study of Pd atoms adsorbed on ultrathin SiO<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML"><mml:msub><mml:mrow /><mml:mn>2</mml:mn></mml:msub></mml:math>films. Physical Review B, 2014, 89, .	1.1	38
256	Theory of Ferromagnetism in Reduced ZrO_{2â€“x} Nanoparticles. ACS Omega, 2018, 3, 5301-5307.	1.6	38
257	Theoretical analysis of the O(1s) binding-energy shifts in alkaline-earth oxides: Chemical or electrostatic contributions. Physical Review B, 1994, 50, 2576-2581.	1.1	37
258	Electronic structure and spectral properties of paramagnetic point defects inSi3N4. Physical Review B, 1999, 60, 12617-12625.	1.1	37
259	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.	1.2	37
260	Pd1/MgO(): a model system in nanocatalysis. Surface Science, 2002, 514, 249-255.	0.8	37
261	Interaction of Ag, Rh, and Pd Atoms with MgO Thin Films Studied by the CO Probe Molecule. Journal of Physical Chemistry B, 2003, 107, 9377-9387.	1.2	37
262	Tailoring the Interaction Strength between Gold Particles and Silica Thin Films via Work Function Control. Physical Review Letters, 2009, 103, 056801.	2.9	37
263	Adsorption of Late Transition Metal Atoms on MgO/Mo(100) and MgO/Ag(100) Ultrathin Films: A Comparative DFT Study. Journal of Physical Chemistry C, 2009, 113, 16694-16701.	1.5	37
264	Fiftyâ€“Fifty Zrâ€“Ti Solid Solution with a TiO₂-Type Structure: Electronic Structure and Photochemical Properties of Zirconium Titanate ZrTiO₄. Journal of Physical Chemistry C, 2017, 121, 5487-5497.	1.5	37
265	Oxideâ€Supported Gold Clusters and Nanoparticles in Catalysis: A Computational Chemistry Perspective. ChemCatChem, 2019, 11, 73-89.	1.8	37
266	Density-functional model cluster studies of EPR g tensors of Fs+ centers on the surface of MgO. Journal of Chemical Physics, 2006, 124, 044708.	1.2	36
267	DFT Study of CO₂ Activation on Doped and Ultrathin MgO Films.. Journal of Physical Chemistry C, 2015, 119, 27594-27602.	1.5	36
268	Evidence of Charge Transfer to Atomic and Molecular Adsorbates on ZnO/X(111) (X = Cu, Ag, Au) Ultrathin Films. Relevance for Cu/ZnO Catalysts. ACS Catalysis, 2018, 8, 4110-4119.	5.5	36
269	Nitrogen doping in coexposed (001)â€“(101) anatase TiO₂ surfaces: a DFT study. Physical Chemistry Chemical Physics, 2019, 21, 21497-21505.	1.3	36
270	On the nature of the bonding in Mg4 and Ca4 clusters. Journal of Chemical Physics, 1982, 77, 5850-5851.	1.2	35

#	Article	IF	Citations
271	Bonding geometry and bonding character of thiocyanate adsorbed on a Ag(100) surface. Journal of Chemical Physics, 1991, 95, 4678-4684.	1.2	35
272	Developing magnetic and metallic behavior in high-nuclearity nickel cluster carbonyls. A LCGTO-LDF study of [Ni9(CO)18]n-, [Ni10Ge(CO)20]n-, [Ni32C6(CO)36]n-, and [Ni44(CO)48]n- compounds. Journal of the American Chemical Society, 1992, 114, 3549-3555.	6.6	35
273	Effects of relativity on the Niî—¸CO, Pdî—¸CO, and Ptî—¸CO bonding mechanism: a constrained space orbital variation analysis of density functional results. Chemical Physics Letters, 1996, 248, 109-115.	1.2	35
274	Adsorption properties of Ni4 and Ni8 clusters supported on regular and defect sites of the MgO (001) surface. Surface Science, 2002, 499, 73-84.	0.8	35
275	Ground- and excited-state properties ofM-center oxygen vacancy aggregates in the bulk and surface of MgO. Physical Review B, 2003, 68, .	1.1	35
276	Optical properties of Cu nanoclusters supported on MgO(100). Journal of Chemical Physics, 2004, 121, 7457-7466.	1.2	35
277	Structure and ESR properties of self-trapped holes in pure silica from first-principles density functional calculations. Physical Review B, 2007, 76, .	1.1	35
278	Nature of Defect States in Nitrogen-Doped MgO. Journal of Physical Chemistry C, 2010, 114, 1350-1356.	1.5	35
279	Conversion of NO to N2O on MgO Thin Films. Journal of Physical Chemistry B, 2002, 106, 7666-7673.	1.2	34
280	A Route toward the Generation of Thermally Stable Au Cluster Anions Supported on the MgO Surface. Journal of the American Chemical Society, 2008, 130, 8690-8695.	6.6	34
281	Hydration Structure of the Ti(III) Cation as Revealed by Pulse EPR and DFT Studies: New Insights into a Textbook Case. Inorganic Chemistry, 2011, 50, 2385-2394.	1.9	34
282	Initial Formation of Positively Charged Gold on MgO(001) Thin Films: Identification by Experiment and Structural Assignment by Theory. Journal of Physical Chemistry C, 2011, 115, 10114-10124.	1.5	34
283	Strain-induced formation of ultrathin mixed-oxide films. Physical Review B, 2011, 83, .	1.1	34
284	Reductant composition influences the coordination of atomically dispersed Rh on anatase TiO₂. Catalysis Science and Technology, 2020, 10, 1597-1601.	2.1	34
285	CO Adsorption on Graphite-like ZnO Bilayers Supported on Cu(111), Ag(111), and Au(111) Surfaces. Journal of Physical Chemistry C, 2017, 121, 27453-27461.	1.5	34
286	Mixed-basis approach to the chemisorption problem; Example of H chemisorption on Lin clusters which model the Li (100) surface. Surface Science, 1984, 144, 602-618.	0.8	33
287	Electronic Effects in the Activation of Supported Metal Clusters:Â Density Functional Theory Study of H2Dissociation on Cu/SiO2. Journal of Physical Chemistry B, 1999, 103, 8552-8557.	1.2	33
288	Theoretical characterization of charge-transfer reactions between N2 and O2 molecules and paramagnetic oxygen vacancies on the MgO surface. Surface Science, 2001, 479, 83-97.	0.8	33

#	Article	IF	Citations
289	Metal/oxide adhesion energies from first-principles. Surface Science, 2002, 520, 3-5.	0.8	33
290	O₂ Activation by Au₅ Clusters Stabilized on Clean and Electron-Rich MgO Stepped Surfaces. Journal of Physical Chemistry C, 2010, 114, 16973-16978.	1.5	33
291	Resolving all atoms of an alkali halide via nanomodulation of the thin NaCl film surface using the Au(111) reconstruction. Physical Review B, 2012, 85, .	1.1	33
292	Turning a Nonreducible into a Reducible Oxide via Nanostructuring: Opposite Behavior of Bulk ZrO₂ and ZrO₂ Nanoparticles Toward H₂ Adsorption. Journal of Physical Chemistry C, 2016, 120, 15329-15337.	1.5	33
293	Halogen ions adsorption at silver and platinum surfaces: A quantum chemical study. Electrochimica Acta, 1996, 41, 2285-2291.	2.6	32
294	Alkali Metal Doping of MgO:Â Mechanisms of Formation of Paramagnetic Surface Centers. Journal of Physical Chemistry B, 2003, 107, 8498-8506.	1.2	32
295	The 17O hyperfine structure of trapped holes photo generated at the surface of polycrystalline MgO. Chemical Physics Letters, 2005, 403, 124-128.	1.2	32
296	Palladium Monomers, Dimers, and Trimers on the MgO(001) Surface Viewed Individually. Angewandte Chemie - International Edition, 2007, 46, 8703-8706.	7.2	32
297	pH Dependent Electronic and Geometric Structures at the Waterâ€“Silica Nanoparticle Interface. Journal of Physical Chemistry C, 2014, 118, 29007-29016.	1.5	32
298	Communication: Hole localization in Al-doped quartz SiO2 within ab initio hybrid-functional DFT. Journal of Chemical Physics, 2015, 143, 111103.	1.2	32
299	Applicability of a pseudopotential CI method to the investigation of ground and excited states of molecular systems: NaCO, Li2H, Al2 and AlH. Theoretica Chimica Acta, 1983, 62, 461-475.	0.9	31
300	Theoretical investigation of the electronic structure and of the potential energy curves for the lowest-lying states of Ge2. Molecular Physics, 1983, 49, 727-736.	0.8	31
301	Low-lying electronic states of Ben clusters (n = 7, 10, 13) and of the Be7î—¸H system. Chemical Physics, 1984, 83, 261-274.	0.9	31
302	Theoretical Aspects of the Electronic Structure and the Stability of Small Clusters. Zeitschrift Fur Elektrotechnik Und Elektrochemie, 1984, 88, 233-238.	0.9	31
303	Electronic structure of nickel carbonyl clusters: chemical bonding and spectroscopy of [Ni5(CO)12]2-, [Ni6(CO)12]2-, and [Ni8C(CO)16]2- studied by the LCGTO-LDF method. Inorganic Chemistry, 1990, 29, 2901-2908.	1.9	31
304	N2-Radical Anion Reversibly Formed at the Surface of â€œElectron-Richâ€•Alkaline-Earth Oxides. Journal of Physical Chemistry B, 2000, 104, 1887-1890.	1.2	31
305	Optical properties of peroxy radicals in silica: Multiconfigurational perturbation theory calculations. Journal of Chemical Physics, 2001, 114, 6259-6264.	1.2	31
306	A Molecular Tool for Measuring the Electron-Acceptor Ability of Ligands from Crystallographic Data. European Journal of Inorganic Chemistry, 2004, 2004, 1705-1713.	1.0	31

#	Article	IF	Citations
307	Evidence for a Sizeâ€Selective Adsorption Mechanism on Oxide Surfaces: Pd and Au atoms on SiO₂/Mo(112). ChemPhysChem, 2008, 9, 1367-1370.	1.0	31
308	F and F⁺ Centers on MgO/Ag(100) or MgO/Mo(100) Ultrathin Films:â€‰ Are They Stable?. Journal of Physical Chemistry C, 2008, 112, 3857-3865.	1.5	31
309	How Growing Conditions and Interfacial Oxygen Affect the Final Morphology of MgO/Ag(100) Films. Journal of Physical Chemistry C, 2014, 118, 26091-26102.	1.5	31
310	Relative stabilities of hydridocarbonyl and formyl complexes of Rh and Pd: A theoretical study. Journal of Catalysis, 1988, 112, 34-43.	3.1	30
311	On the origin of the 5.0 and 7.6 eV absorption bands in oxygen deficient Î±-quartz and amorphous silica. A first principles quantum-chemical study. Journal of Non-Crystalline Solids, 1997, 216, 1-9.	1.5	30
312	Interaction of H2 with strained rings at the silica surface from ab initio calculations. Journal of Non-Crystalline Solids, 2000, 271, 56-63.	1.5	30
313	Oâ˜ radical anions on polycrystalline MgO. Surface Science, 2002, 521, 104-116.	0.8	30
314	Nucleation and growth of Ni clusters on regular sites and F centers on the MgO() surface. Surface Science, 2003, 522, 175-184.	0.8	30
315	Reactivity of (H+)(eâ˜) color centers at the MgO surface: formation of O2â˜ and N2â˜ radical anions. Surface Science, 2003, 542, 293-306.	0.8	30
316	Theory of oxides surfaces, interfaces and supported nano-clusters. Theoretical Chemistry Accounts, 2007, 117, 827-845.	0.5	30
317	Li, Al, and Ni Substitutional Doping in MgO Ultrathin Films on Metals: Work Function Tuning via Charge Compensation. Journal of Physical Chemistry C, 2012, 116, 5781-5786.	1.5	30
318	Theoretical investigation of the interaction between the hydrogen atom and Pd clusters. Surface Science, 1985, 154, 126-138.	0.8	29
319	Analysis of the bonding mechanism of benzene on Cu(110), Cu(111), Pd(111) and the effect of coadsorbed C1 atoms. Surface Science, 1996, 365, 297-309.	0.8	29
320	Structure of ultrathin crystallineSiO2films on Mo(112). Physical Review B, 2004, 69, .	1.1	29
321	Chemistry on single atoms: key factors for the acetylene trimerization on MgO-supported Rh, Pd, and Ag atoms. Chemical Physics Letters, 2004, 399, 266-270.	1.2	29
322	Observable consequences of formation of Au anions from deposition of Au atoms on ultrathin oxide films. Journal of Chemical Physics, 2007, 127, 144713.	1.2	29
323	Properties of Alkali Metal Atoms Deposited on a MgO Surface: A Systematic Experimental and Theoretical Study. Chemistry - A European Journal, 2008, 14, 4404-4414.	1.7	29
324	Adsorption of Au and Pd Atoms on Thin SiO₂ Films:â€‰ the Role of Atomic Structure. Journal of Physical Chemistry C, 2008, 112, 3405-3409.	1.5	29

#	Article	IF	Citations
325	CO Adsorption on One-, Two-, and Three-Dimensional Au Clusters Supported on MgO/Ag(001) Ultrathin Films. Journal of Physical Chemistry C, 2009, 113, 10256-10263.	1.5	29
326	Direct Measurement of the Attractive Interaction Forces on F⁰ Color Centers on MgO(001) by Dynamic Force Microscopy. ACS Nano, 2010, 4, 2510-2514.	7.3	29
327	CO+NO versus CO+O₂ Reaction on Monolayer FeO(111) Films on Pt(111). ChemCatChem, 2011, 3, 671-674.	1.8	29
328	Carbothermal Transformation of TiO₂ into TiO_xC_y in UHV: Tracking Intrinsic Chemical Stabilities. Journal of Physical Chemistry C, 2014, 118, 22601-22610.	1.5	29
329	CO adsorption on a silica bilayer supported on Ru(0001). Surface Science, 2016, 648, 2-9.	0.8	29
330	Trends in Adhesion Energies of Gold on MgO(100), Rutile TiO₂(110), and CeO₂(111) Surfaces: A Comparative DFT Study. Journal of Physical Chemistry C, 2017, 121, 28328-28338.	1.5	29
331	On the ground-state properties of the germanium dimer. Chemical Physics Letters, 1984, 107, 70-71.	1.2	28
332	Spin states and quenching of magnetism in naked and carbonylated nickel clusters. Chemical Physics Letters, 1987, 134, 407-412.	1.2	28
333	Five-coordinate platinum (II) alkyne complexes: synthesis, ab initio calculations and crystal and molecular structure of [PtI2(Me2phen)Î·2PhCî—¼CPh]Â·CHCl3. Inorganica Chimica Acta, 1998, 275-276, 500-509.	1.2	28
334	Title is missing!. Topics in Catalysis, 1999, 9, 153-161.	1.3	28
335	Analysis of electronic contributions to the vibrational frequency of CO/Cu2O(111). Surface Science, 1999, 430, 137-145.	0.8	28
336	Local Environment of Electrons Trapped at the MgO Surface:â€‰ Spin Density on the Oxygen Ions from 17O Hyperfine Coupling Constants. Journal of Physical Chemistry B, 2004, 108, 11529-11534.	1.2	28
337	Nature of Point Defects on SiO2/Mo(112) Thin Films and Their Interaction with Au Atoms. Journal of Physical Chemistry B, 2006, 110, 17015-17023.	1.2	28
338	Partially Hydroxylated Polycrystalline Ionic Oxides:Â A New Route toward Electron-Rich Surfaces. Journal of the American Chemical Society, 2007, 129, 10575-10581.	6.6	28
339	Electronic structure of Al, Ga, In and Cu doped ZnO/Cu(111) bilayer films. Physical Chemistry Chemical Physics, 2019, 21, 369-377.	1.3	28
340	Metal-metal bonding in free and ligated nickel clusters. Inorganic Chemistry, 1993, 32, 2963-2964.	1.9	27
341	Core-level binding-energy shifts due to ionic adsorbates. Physical Review B, 1993, 48, 15262-15273.	1.1	27
342	Ionic and covalent electronic states for K adsorbed on Cu5 and Cu25 cluster models of the Cu(100) surface. Journal of Chemical Physics, 1995, 102, 879-887.	1.2	27

#	Article	IF	Citations
343	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.	1.9	27
344	Calculated spectral properties of self-trapped holes in pure and Ge-dopedSiO2. Physical Review B, 1999, 60, 9990-9998.	1.1	27
345	Simplified embedding schemes for the quantum-chemical description of neutral and charged point defects in SiO2 and related dielectrics. Journal of Chemical Physics, 2000, 113, 10744-10752.	1.2	27
346	A Theoretical Study of Catalytic Coupling of Propyne on Cu{111}. Journal of the American Chemical Society, 2000, 122, 7573-7578.	6.6	27
347	Cluster and periodic ab initio calculations on the adsorption of CO2 on the SnO2(110) surface. Surface Science, 2001, 478, 25-34.	0.8	27
348	X-ray Photoemission Study of the Charge State of Au Nanoparticles on Thin MgO/Fe(001) Films. Journal of Physical Chemistry C, 2009, 113, 19957-19965.	1.5	27
349	Unraveling the atomic structure, ripening behavior, and electronic structure of supported Au ₂₀ clusters. Science Advances, 2020, 6, eaay4289.	4.7	27
350	Charge transfer effects and photoemission in transition metal oxides. Chemical Physics Letters, 1996, 251, 90-94.	1.2	26
351	Adsorption of NO and NO2 on terrace and step sites and on oxygen vacancies of the CaO(100) surface. Surface Science, 2004, 556, 145-158.	0.8	26
352	Radical versus Nucleophilic Mechanism of Formaldehyde Polymerization Catalyzed by (WO3)3 Clusters on Reduced or Stoichiometric TiO2(110). Journal of the American Chemical Society, 2012, 134, 14086-14098.	6.6	26
353	Plasmonic Au nanoclusters dispersed in nitrogen-doped graphene as a robust photocatalyst for light-to-hydrogen conversion. Journal of Materials Chemistry A, 2021, 9, 22810-22819.	5.2	26
354	Low-lying states and electronic structures of Sn2and Pb2molecules. Molecular Physics, 1985, 55, 211-223.	0.8	25
355	Does the electronegativity scale apply to ionic crystals as to molecules? A theoretical study of the bonding character in molecular and crystalline alkaline-earth oxides based on dipole moments. Chemical Physics, 1995, 199, 155-162.	0.9	25
356	Nano-assembled Pd catalysts on MgO thin films. Thin Solid Films, 2001, 400, 37-42.	0.8	25
357	Formation of Pd dimers at regular and defect sites of the MgO(100) surface: cluster model calculations. Chemical Physics, 2005, 309, 41-47.	0.9	25
358	Vibrational and electron paramagnetic resonance properties of free and MgO supported AuCO complexes. Journal of Chemical Physics, 2006, 124, 174709.	1.2	25
359	Li atoms deposited on single crystalline MgO(001) surface. A combined experimental and theoretical study. Chemical Physics Letters, 2008, 450, 308-311.	1.2	25
360	Realization of an atomic sieve: Silica on Mo(112). Surface Science, 2009, 603, 1145-1149.	0.8	25

#	Article	IF	Citations
361	Atomic Scale Structure and Reduction of Cerium Oxide at the Interface with Platinum. Advanced Materials Interfaces, 2015, 2, 1500375.	1.9	25
362	CO2 Activation and Hydrogenation: A Comparative DFT Study of Ru10/TiO2 and Cu10/TiO2 Model Catalysts. Catalysis Letters, 2017, 147, 1871-1881.	1.4	25
363	Ultrathin silica films on Pd(111): Structure and adsorption properties. Surface Science, 2018, 678, 118-123.	0.8	25
364	Solar-driven chemistry: towards new catalytic solutions for a sustainable world. Rendiconti Lincei, 2019, 30, 443-452.	1.0	25
365	Charge Carriers Cascade in a Ternary TiO₂/TiO₂/ZnS Heterojunction: A DFT Study. ChemCatChem, 2020, 12, 2097-2105.	1.8	25
366	Z-Scheme versus type-II junction in g-C₃N₄/TiO₂ and g-C₃N₄/SrTiO₃/TiO₂ heterostructures. Catalysis Science and Technology, 2021, 11, 3589-3598.	2.1	25
367	The adsorption of CO on : a joint experimental and theoretical study. Surface Science, 1995, 330, 156-172.	0.8	24
368	Adsorption complexes on oxides: Density functional model cluster studies. Theoretical and Computational Chemistry, 1996, , 569-619.	0.2	24
369	FS+ and FS+(OHâ^') defect centers at the MgO(100) surface: cluster and periodic calculations. Surface Science, 2004, 549, 294-304.	0.8	24
370	EPR properties of Au atoms adsorbed on various sites of the MgO(100) surface from relativistic DFT calculations. Surface Science, 2006, 600, 2434-2442.	0.8	24
371	Electron Traps on Oxide Surfaces: (H+)(eâ^') Pairs Stabilized on the Surface of 17O Enriched CaO. ChemPhysChem, 2006, 7, 728-734.	1.0	24
372	Controlling the charge state of single Mo dopants in a CaO film. Physical Review B, 2013, 88, .	1.1	24
373	Electrostatic and chemical bonding contributions to the cation core level binding energy shifts in MgO, CaO, SrO, BaO. A cluster model study. Journal of Electron Spectroscopy and Related Phenomena, 1993, 63, 189-205.	0.8	23
374	Ionicity of alkali-metal adsorbates. Physical Review Letters, 1993, 71, 206-206.	2.9	23
375	Electronic Structure of Defect Centers P1, P2, and P4 in P-Doped SiO2. Journal of Physical Chemistry B, 2001, 105, 6097-6102.	1.2	23
376	Electronic Structure and Reactivity of the FS(H)+ Defect Center at the MgO (001) Surface. Journal of Physical Chemistry B, 2001, 105, 9798-9804.	1.2	23
377	Interaction of CO, CO2 and CH4 with mesoporous organosilica: Periodic DFT calculations with dispersion corrections. Microporous and Mesoporous Materials, 2010, 129, 62-67.	2.2	23
378	Self-Doping of Ultrathin Insulating Films by Transition Metal Atoms. Physical Review Letters, 2014, 112, 026102.	2.9	23

#	Article	IF	Citations
379	Magnetic properties of nitrogen-doped ZrO2: Theoretical evidence of absence of room temperature ferromagnetism. Scientific Reports, 2016, 6, 31435.	1.6	23
380	Nature of SrTiO3/TiO2 (anatase) heterostructure from hybrid density functional theory calculations. Journal of Chemical Physics, 2020, 152, 184704.	1.2	23
381	On the Real Nature of Rh Singleâ€Atom Catalysts Dispersed on the ZrO₂ Surface. ChemCatChem, 2020, 12, 2595-2604.	1.8	23
382	The importance of correlation effects on the bonding of atomic oxygen on Pt(111). Journal of Chemical Physics, 1996, 105, 7192-7199.	1.2	22
383	On the origin of bonding and vibrational frequency shifts for CO adsorbed on neutral, cationic and anionic gold clusters. Journal of Physics: Conference Series, 2008, 117, 012003.	0.3	22
384	A DFT study of Ni clusters deposition on titania and zirconia (101) surfaces. Surface Science, 2016, 646, 230-238.	0.8	22
385	Influence of surface hydroxylation on the Ru atom diffusion on the ZrO2(101) surface: A DFT study. Surface Science, 2017, 664, 87-94.	0.8	22
386	Band Gap in Magnetic Insulators from a Charge Transition Level Approach. Journal of Chemical Theory and Computation, 2020, 16, 3786-3798.	2.3	22
387	WO₃/BiVO₄ Photoanodes: Facets Matching at the Heterojunction and BiVO₄ Layer Thickness Effects. ACS Applied Energy Materials, 2021, 4, 8421-8431.	2.5	22
388	Bonding of transition metal atoms on the Al(100) surface from density functional calculations. Surface Science, 1998, 412-413, 616-624.	0.8	21
389	Mechanisms of Proton Formation from Interaction of H2with Eâ€˜ and Oxygen Vacancy Centers in SiO2:Â Cluster Model Calculations. Journal of Physical Chemistry B, 2000, 104, 5471-5477.	1.2	21
390	Modifying the Adsorption Characteristic of Inert Silica Films by Inserting Anchoring Sites. Physical Review Letters, 2009, 102, 016102.	2.9	21
391	Lithium incorporation into a silica thin film: Scanning tunneling microscopy and density functional theory. Physical Review B, 2009, 80, .	1.1	21
392	A DFT Study of the Reactivity of Anatase TiO₂ and Tetragonal ZrO₂ Stepped Surfaces Compared to the Regular (101) Terraces. ChemPhysChem, 2015, 16, 3642-3651.	1.0	21
393	Theoretical description of metal/oxide interfacial properties: The case of MgO/Ag(001). Applied Surface Science, 2016, 390, 578-582.	3.1	21
394	pH Dependence of MgO, TiO₂, and Î³-Al₂O₃ Surface Chemistry from First Principles. Journal of Physical Chemistry C, 2022, 126, 10216-10223.	1.5	21
395	Promotion by alkali metals: a theoretical analysis of the vibrational shift of CO coadsorbed with K on Cu(100). Chemical Physics, 1993, 177, 373-385.	0.9	20
396	Charge transfer and charge conversion ofKandNdefect centers inSi3N4. Physical Review B, 2000, 61, 15005-15010.	1.1	20

#	Article	IF	Citations
397	Local zero-bias anomaly in tunneling spectra of a transition-metal oxide thin film. Physical Review B, 2007, 75, .	1.1	20
398	DFT Simulations of Titanium Oxide Films on Titanium Metal. Journal of Physical Chemistry C, 2013, 117, 358-367.	1.5	20
399	Properties of two-dimensional insulators: a DFT study of Co adsorption on NaCl and MgO ultrathin films. Physical Chemistry Chemical Physics, 2014, 16, 21838-21845.	1.3	20
400	Adsorption of Benzene on Cu(100) and on Cu(100) Covered with an Ultrathin NaCl Film: Moleculeâ€“Substrate Interaction and Decoupling. Journal of Physical Chemistry C, 2015, 119, 4062-4071.	1.5	20
401	Characterization of Acid and Basic Sites on Zirconia Surfaces and Nanoparticles by Adsorbed Probe Molecules: A Theoretical Study. Topics in Catalysis, 2020, 63, 1717-1730.	1.3	20
402	Role of surface termination and quantum size in Î±-CsPbX₃ (X = Cl, Br, I) 2D nanostructures for solar light harvesting. Physical Chemistry Chemical Physics, 2021, 23, 3031-3040.	1.3	20
403	Nature and Role of Surface Junctions in BiOIO₃ Photocatalysts. Advanced Functional Materials, 2021, 31, 2009472.	7.8	20
404	Coordination of boron and phosphorous in borophosphosilicate glasses. Applied Physics Letters, 2003, 83, 4312-4314.	1.5	19
405	Catalytic dissociation of N2O on pure and Ni-doped MgO surfaces. Surface Science, 2006, 600, 386-394.	0.8	19
406	Identification of Active Sites in a Realistic Model of Strong Metalâ€“Support Interaction Catalysts: The Case of Platinumâ€‰(1â€‰1â€‰1)â€Supported Iron Oxide Film. ChemCatChem, 2014, 6, 185-190.	1.8	19
407	Surface defects and their impact on the electronic structure of Mo-doped CaO films: an STM and DFT study. Physical Chemistry Chemical Physics, 2014, 16, 12764-12772.	1.3	19
408	Properties of Pt-supported iron oxide ultra-thin films: Similarity of Hubbard-corrected and hybrid density functional theory description. Journal of Chemical Physics, 2014, 141, 144702.	1.2	19
409	Reducibility of ZrO₂/Pt₃Zr and ZrO₂/Pt 2D films compared to bulk zirconia: a DFT+U study of oxygen removal and H₂adsorption. Nanoscale, 2017, 9, 6866-6876.	2.8	19
410	CO Oxidation Promoted by a Pt4/TiO2 Catalyst: Role of Lattice Oxygen at the Metal/Oxide Interface. Catalysis Letters, 2019, 149, 390-398.	1.4	19
411	Band offset in semiconductor heterojunctions. Journal of Physics Condensed Matter, 2021, 33, 415002.	0.7	19
412	Electronic structure and reactivity of the transition-metal lithides ScLi, CuLi and PdLi. Chemical Physics Letters, 1985, 116, 423-428.	1.2	18
413	CO adsorption on Ni4 and Ni8 clusters deposited on regular and defect sites of the MgO(001) surface. Surface Science, 2005, 575, 103-114.	0.8	18
414	Tuning the Charge State of (WO₃)₃ Nanoclusters Deposited on MgO/Ag(001) Films. Journal of Physical Chemistry C, 2012, 116, 17668-17675.	1.5	18

#	Article	IF	Citations
415	Nature of Paramagnetic Species in Nitrogen-Doped SnO₂: A Combined Electron Paramagnetic Resonance and Density Functional Theory Study. Journal of Physical Chemistry C, 2015, 119, 26895-26903.	1.5	18
416	Ferromagnetic Interactions in Highly Stable, Partially Reduced TiO₂: The S=2 State in Anatase. Angewandte Chemie - International Edition, 2017, 56, 2604-2607.	7.2	18
417	Oxygen Vacancy in Wurtzite ZnO and Metal-Supported ZnO/M(111) Bilayer Films (M = Cu, Ag and Au). Journal of Physical Chemistry C, 2018, 122, 20880-20887.	1.5	18
418	Role of surface termination in forming type-II photocatalyst heterojunctions: the case of TiO₂/BiVO₄. Journal of Physics Condensed Matter, 2021, 33, 075001.	0.7	18
419	Quantum chemical modelling case studies relevant to metal oxide dissolution and catalysis. Ionics, 2001, 7, 290-309.	1.2	17
420	Charging and stabilization of Pd atoms and clusters on an electron-rich MgO surface. Surface Science, 2008, 602, 2801-2807.	0.8	17
421	Formation of Superoxo Species by Interaction of O₂ with Na Atoms Deposited on MgO Powders: A Combined Continuousâ€Wave EPR (CWâ€EPR), Hyperfine Sublevel Correlation (HYSCORE) and DFT Study. Chemistry - A European Journal, 2010, 16, 6776-6785.	1.7	17
422	Lateral Manipulation of Atomic Vacancies in Ultrathin Insulating Films. ACS Nano, 2015, 9, 5318-5325.	7.3	17
423	Bending Rigidity of 2D Silica. Physical Review Letters, 2018, 120, 226101.	2.9	17
424	Origin of the Ba core-level binding-energy difference between tetragonal and orthorhombicYBa2Cu3O7âˆ’Î´. Physical Review B, 1991, 43, 3695-3698.	1.1	16
425	Surface-bulk core-level binding-energy shifts for Al(100). Physical Review B, 1993, 48, 15274-15282.	1.1	16
426	Microscopic mechanisms of radiation-induced proton density decay in SiO/sub 2/ films. IEEE Transactions on Nuclear Science, 1998, 45, 2408-2412.	1.2	16
427	29Si solid state NMR of hydroxyl groups in silica from first principle calculations. Materials Science and Engineering B: Solid-State Materials for Advanced Technology, 1999, 68, 16-21.	1.7	16
428	Cu atoms and clusters on regular and defect sites of the SiO2 surface. Electronic structure and properties from first principle calculations. Faraday Discussions, 1999, 114, 209-222.	1.6	16
429	Bonding of NO on NixMg1âˆ’xO powders: an EPR and computational study. Journal of Molecular Catalysis A, 2003, 204-205, 779-786.	4.8	16
430	Theoretical modeling of photon- and electron-stimulated Na and K desorption fromSiO2. Physical Review B, 2004, 69, .	1.1	16
431	Cluster and Periodic DFT Calculations of MgO/Pd(CO) and MgO/Pd(CO)2Surface Complexes. Journal of Physical Chemistry B, 2005, 109, 3416-3422.	1.2	16
432	Methanol Oxidation Reaction on Î±â€Tungsten Carbide Versus Platinum (1â€‰1â€‰1) Surfaces: A DFT Electrochemical Study. ChemCatChem, 2015, 7, 3533-3543.	1.8	16

#	Article	IF	Citations
433	Atomic structure of a metal-supported two-dimensional germania film. Physical Review B, 2018, 97, .	1.1	16
434	TiO ₂ and ZrO ₂ in biomass conversion: why catalyst reduction helps. Philosophical Transactions Series A, Mathematical, Physical, and Engineering Sciences, 2018, 376, 20170056.	1.6	16
435	Theoretical treatment of semiconductor heterojunctions for photocatalysis: the WO₃/BiVO₄ interface. Journal of Physics Condensed Matter, 2019, 31, 434001.	0.7	16
436	Nature of Atomically Dispersed Ru on Anatase TiO₂: Revisiting Old Data Based on DFT Calculations. Journal of Physical Chemistry C, 2019, 123, 7271-7282.	1.5	16
437	Electronic structure of metal carbonyl clusters. 2. An INDO investigation of tetra-, penta-, and hexanuclear nickel complexes. Inorganic Chemistry, 1984, 23, 247-253.	1.9	15
438	Bonding of water ligands to copper and nickel atoms: crucial role of intermolecular electron correlation. The Journal of Physical Chemistry, 1986, 90, 3051-3052.	2.9	15
439	Role of surface heterogeneity in the chemical bond of MgO: ionic character of regular and defect surface sites. Chemical Physics Letters, 1996, 249, 123-129.	1.2	15
440	Structure and properties of dimer, trimer and tetramer aggregates of methyltrioxorhenium (MTO): an ab initio study. Journal of Organometallic Chemistry, 1996, 514, 111-117.	0.8	15
441	First principle calculations of the optical properties of a neutral oxygen vacancy in Ge-doped silica. Journal of Non-Crystalline Solids, 1999, 254, 17-25.	1.5	15
442	Theory of point defects at the MgO surface. Chemical Physics of Solid Surfaces, 2001, , 94-135.	0.3	15
443	Ab Initio Molecular Dynamics Simulation of NO Reactivity on the CaO(001) Surface. Journal of Physical Chemistry B, 2006, 110, 8357-8362.	1.2	15
444	Adsorption of transition metal atoms on the NiO(100) surface and on NiO/Ag(100) thin films. Theoretical Chemistry Accounts, 2008, 120, 575-582.	0.5	15
445	Gold Nanostructures on TiOx/Mo(112) Thin Films. Journal of Physical Chemistry C, 2008, 112, 191-200.	1.5	15
446	Spontaneous Oxidation of Ni Nanoclusters on MgO Monolayers Induced by Segregation of Interfacial Oxygen. Journal of Physical Chemistry Letters, 2015, 6, 3104-3109.	2.1	15
447	Spontaneous doping of two-dimensional NaCl films with Cr atoms: aggregation and electronic structure. Nanoscale, 2015, 7, 2366-2373.	2.8	15
448	ZrO2 Nanoparticles: a density functional theory study of structure, properties and reactivity. Rendiconti Lincei, 2017, 28, 19-27.	1.0	15
449	Layered oxides as cathode materials for beyond-Li batteries: A computational study of Ca and Al intercalation in bulk V2O5 and MoO3. Computational Materials Science, 2021, 191, 110324.	1.4	15
450	Steric and Orbital Effects Induced by Isovalent Dopants on the Surface Chemistry of ZrO2. ACS Catalysis, 2021, 11, 554-567.	5.5	15

#	Article	IF	Citations
451	Electronic and magnetic properties of organometallic clusters: From the molecular to the metallic state. International Journal of Quantum Chemistry, 1992, 44, 605-619.	1.0	14
452	The reactivity of CO2 with K atoms adsorbed on MgO powders. Physical Chemistry Chemical Physics, 2009, 11, 8156.	1.3	14
453	Mechanism of Charging of Au Atoms and Nanoclusters on Li Doped SiO₂/Mo(112) Films. ChemPhysChem, 2010, 11, 412-418.	1.0	14
454	Dopant-Induced Diffusion Processes at Metalâ€“Oxide Interfaces Studied for Iron- and Chromium-Doped MgO/Mo(001) Model Systems. Journal of Physical Chemistry C, 2016, 120, 13604-13609.	1.5	14
455	Reduction of Hydrogenated ZrO₂ Nanoparticles by Water Desorption. ACS Omega, 2017, 2, 3878-3885.	1.6	14
456	Reduced sintering of mass-selected Au clusters on SiO₂by alloying with Ti: an aberration-corrected STEM and computational study. Nanoscale, 2018, 10, 2363-2370.	2.8	14
457	Formation of Reversible Adducts by Adsorption of Oxygen on Ceâ€“ZrO₂: An Unusual Î·² Ionic Superoxide. Journal of Physical Chemistry C, 2019, 123, 27088-27096.	1.5	14
458	Role of Metal/Oxide Interfaces in Enhancing the Local Oxide Reducibility. Topics in Catalysis, 2019, 62, 1192-1201.	1.3	14
459	Determination of Silica and Germania Film Network Structures on Ru(0001) at the Atomic Scale. Journal of Physical Chemistry C, 2019, 123, 7889-7897.	1.5	14
460	Cluster Catalysis with Lattice Oxygen: Tracing Oxygen Transport from a Magnetite (001) Support onto Small Pt Clusters. ACS Catalysis, 2021, 11, 9519-9529.	5.5	14
461	LaFeO₃ meets nitrogen-doped graphene functionalized with ultralow Pt loading in an impactful Z-scheme platform for photocatalytic hydrogen evolution. Journal of Materials Chemistry A, 2022, 10, 3330-3340.	5.2	14
462	The electronic structure of carbonyl metal clusters. Journal of Organometallic Chemistry, 1982, 224, 89-105.	0.8	13
463	Potential energy surfaces of low-lying states of the aluminum trimer. Chemical Physics Letters, 1987, 142, 85-91.	1.2	13
464	Adsorption of CS2 on MgO microcrystals: formation of a S-doped MgO surface. Physical Chemistry Chemical Physics, 2002, 4, 366-374.	1.3	13
465	Adsorption of Li, Na, K, and Mg Atoms on Amorphous and Crystalline Silica Bilayers on Ru(0001): A DFT Study. Journal of Physical Chemistry C, 2014, 118, 15884-15891.	1.5	13
466	Effect of Nanostructuring on the Reactivity of Zirconia: A DFT+U Study of Au Atom Adsorption. Journal of Physical Chemistry C, 2016, 120, 17604-17612.	1.5	13
467	Adsorption and Dimerization of Late Transition Metal Atoms on the Regular and Defective Quartz (001) Surface. Topics in Catalysis, 2017, 60, 459-470.	1.3	13
468	Growth and Atomicâ€Scale Characterization of Ultrathin Silica and Germania Films: The Crucial Role of the Metal Support. Chemistry - A European Journal, 2021, 27, 1870-1885.	1.7	13

#	Article	IF	Citations
469	CO Chemisorption on Oxide Surfaces: Bonding and Vibrations. NATO ASI Series Series B: Physics, 1992, , 305-320.	0.2	13
470	Growth of Nâ€Heterocyclic Carbene Assemblies on Cu(100) and Cu(111): From Single Molecules to Magicâ€Number Islands. Angewandte Chemie - International Edition, 2022, 61, .	7.2	13
471	Cluster-model study of the interaction of halogen atoms with Ag clusters. Zeitschrift FÃ¼r Physik D-Atoms Molecules and Clusters, 1989, 12, 543-546.	1.0	12
472	In situ vibrational spectroscopy of contact adsorbed thiocyanate on silver electrodes: experiment and theory. Langmuir, 1991, 7, 1261-1268.	1.6	12
473	Bonding of vinylidene on Pd(111). Computational and Theoretical Chemistry, 1998, 458, 123-129.	1.5	12
474	Infra-red, electron paramagnetic resonance and X-ray photoemission spectral properties of point defects in silica from first-principle calculations. Journal of Non-Crystalline Solids, 1999, 245, 175-182.	1.5	12
475	Electronic structure of the paramagnetic boron oxygen hole center in B-dopedSiO2. Physical Review B, 2001, 64, .	1.1	12
476	Phosphorousâ€“oxygen hole centers in phosphosilicate glass films. Physical Review B, 2006, 74, .	1.1	12
477	A DFT study of PtAu bimetallic clusters adsorbed on MgO/Ag(100) ultrathin films. Physical Chemistry Chemical Physics, 2010, 12, 6352.	1.3	12
478	Phonon-Mediated Electron Transport through CaO Thin Films. Physical Review Letters, 2015, 114, 016804.	2.9	12
479	Size-Dependent Penetration of Gold Nanoclusters through a Defect-Free, Nonporous NaCl Membrane. Nano Letters, 2016, 16, 3063-3070.	4.5	12
480	Spontaneous Formation of Gold Cluster Anions on ZnO/Cu(111) Bilayer Films. Journal of Physical Chemistry C, 2019, 123, 7644-7653.	1.5	12
481	Fast atom bombardment mass spectrometry of ionic gold(I) and gold(III) carbene derivatives: An investigation of the formation of [M - H]+ species. Organic Mass Spectrometry, 1991, 26, 945-950.	1.3	11
482	Structure, Composition, and Electronic Properties of TiOx/Mo(112) Thin Films. Journal of Physical Chemistry C, 2007, 111, 7437-7445.	1.5	11
483	Stabilizing Monomeric Iron Species in a Porous Silica/Mo(112) Film. ACS Nano, 2010, 4, 863-868.	7.3	11
484	Spectroscopic Evidences of Charge Transfer Phenomena and Stabilization of Unusual Phases at Iron Oxide Monolayers Grown on Pt(111). Topics in Catalysis, 2013, 56, 1074-1081.	1.3	11
485	The photoactive nitrogen impurity in nitrogen-doped zirconium titanate (N-ZrTiO4): a combined electron paramagnetic resonance and density functional theory study. Journal of Materials Chemistry A, 2017, 5, 13062-13071.	5.2	11
486	The epitaxial growth of ZnO films on Cu(111) surface: Thickness dependence. Applied Surface Science, 2019, 483, 133-139.	3.1	11

#	Article	IF	Citations
487	Structural, electronic and photochemical properties of cerium-doped zirconium titanate. Catalysis Today, 2020, 340, 49-57.	2.2	11
488	Adsorption and Reaction of CO and CO2 at the Surface and Defect Sites of MgO and NiO. Springer Series in Surface Sciences, 1993, , 180-191.	0.3	11
489	NO adsorption on the stoichiometric and reduced SnO2(110) surface. Theoretical Chemistry Accounts, 2005, 114, 52-59.	0.5	10
490	Comment on â€œThe structure of monolayer SiO2 on Mo(112): A 2-D [Siâ€“Oâ€“Si] network or isolated [SiO4] units?â€• Surface Science, 2007, 601, 588-590.	0.8	10
491	Staying put. Nature Materials, 2009, 8, 167-168.	13.3	10
492	N₂^{â^’} Radical Anions Trapped in Bulk Polycrystalline MgO. Journal of Physical Chemistry C, 2010, 114, 5187-5192.	1.5	10
493	From Crystalline to Amorphous Germania Bilayer Films at the Atomic Scale: Preparation and Characterization. Angewandte Chemie - International Edition, 2019, 58, 10903-10908.	7.2	10
494	The Overproduction of Truth. , 2018, , .		10
495	DFT study of electronic properties of N-doped ZnO and ZnO/Cu(111) bilayer films. Surface Science, 2022, 716, 121978.	0.8	10
496	Transition metal atom-water complexes: A quantum chemical study including electron correlation. Computational and Theoretical Chemistry, 1987, 149, 297-309.	1.5	9
497	Cluster model approach to chemisorption on aluminum: Surface relaxation effects on the interaction of atomic oxygen with the Al(111) surface. Surface Science, 1988, 204, 587-604.	0.8	9
498	Adsorption of Ethyne on Cu(110):â€‰ Experimental and Theoretical Study. Langmuir, 1997, 13, 758-764.	1.6	9
499	The treatment of the spin coupling in the bonding of NO to the Ni-doped MgO (100) surface. Molecular Physics, 2003, 101, 241-247.	0.8	9
500	Probing the Basicity of Regular and Defect Sites of Alkaline Earth Metal Oxide Surfaces by BF3 Adsorption: A Theoretical Analysis. ChemPhysChem, 2004, 5, 642-651.	1.0	9
501	Twoâ€Ðimensional Oxides and Their Role in Electron Transfer Mechanisms with Adsorbed Species. Chemical Record, 2014, 14, 910-922.	2.9	9
502	Anchoring Small Au Clusters on the Dehydroxylated and Hydroxylated SiO2 Î±-Quartz (001) Surface via Ti-Alloying. Journal of Physical Chemistry C, 2017, 121, 14717-14724.	1.5	9
503	Support effects and reaction mechanism of acetylene trimerization over silica-supported Cu 4 clusters: A DFT study. Surface Science, 2018, 668, 125-133.	0.8	9
504	Hydrogen Adsorption on Free-Standing and Agâ€“Pt Supported TiO₂ Thin Films. Journal of Physical Chemistry C, 2019, 123, 7952-7960.	1.5	9

#	Article	IF	Citations
505	Structure of a Silica Thin Film on Oxidized Cu(111): Conservation of the Honeycomb Lattice and Role of the Interlayer. Journal of Physical Chemistry C, 2020, 124, 20942-20949.	1.5	9
506	Bonding Properties of Isolated Metal Atoms on Two-Dimensional Oxides. Journal of Physical Chemistry C, 2020, 124, 20960-20973.	1.5	9
507	Bonding and adsorbate core level shifts of transition metal atoms on the Al(100) surface from density functional calculations. Chemical Physics Letters, 1999, 299, 137-144.	1.2	8
508	DFT Study of 17O NMR Spectroscopy Applied to Zirconia Surfaces and Nanoparticles. Journal of Physical Chemistry C, 2019, 123, 21629-21638.	1.5	8
509	Electronic structure of CuWO₄: dielectric-dependent, self-consistent hybrid functional study of a Mottâ€“Hubbard type insulator. Journal of Physics Condensed Matter, 2019, 31, 145503.	0.7	8
510	H₂ Adsorption on Wurtzite ZnO and on ZnO/M(111) (M=Cu, Ag and Au) Bilayer Films. ChemNanoMat, 2019, 5, 932-939.	1.5	8
511	17O NMR as a measure of basicity of alkaline-earth oxide surfaces: A theoretical study. Journal of Chemical Physics, 2019, 151, 224705.	1.2	8
512	Role of Nanostructuring on the Properties of Oxide Materials: The Case of Zirconia Nanoparticles. European Journal of Inorganic Chemistry, 2019, 2019, 751-761.	1.0	8
513	Applied vs fundamental research in heterogeneous photocatalysis: problems and perspectives. An introduction to â€¯physical principles of photocatalysisâ€™. Journal of Physics Condensed Matter, 2020, 32, 360301.	0.7	8
514	Vibrational Properties of CO Adsorbed on Au Single Atom Catalysts on TiO2(101), ZrO2(101), CeO2(111), and LaFeO3(001) Surfaces: A DFT Study. Topics in Catalysis, 0, , 1.	1.3	8
515	The electronic structure of small metallic clusters. Part III. AB initio calculations of the interaction of atomic hydrogen with small Lin (n = 3, 4, 5) clusters. Journal of Molecular Catalysis, 1981, 12, 245-252.	1.2	7
516	Theoretical INDO Investigation of the Electronic Structure of Aluminium Clusters. Physica Status Solidi (B): Basic Research, 1989, 153, 193-205.	0.7	7
517	First Evidence of a Single-Ion Electron Trap at the Surface of an Ionic Oxide. Angewandte Chemie, 2003, 115, 1801-1803.	1.6	7
518	Reactivity of low-coordinated MgO anions towards CO: A DFT study of (CnOn+1)2â^' polymeric species. Surface Science, 2005, 591, 70-89.	0.8	7
519	Formation of Cationic Gold Clusters on the MgO Surface from Au(CH3)2(acac) Organometallic Precursors:â€‰ A Theoretical Analysis. Journal of Physical Chemistry C, 2007, 111, 5154-5161.	1.5	7
520	Enhanced magnetic moments of Fe clusters supported on MgO/Fe(001) ultrathin films. Journal of Chemical Physics, 2009, 130, 184711.	1.2	7
521	Adsorption Properties of Two-Dimensional NaCl: A Density Functional Theory Study of the Interaction of Co, Ag, and Au Atoms with NaCl/Au(111) Ultrathin Films. Journal of Physical Chemistry C, 2014, 118, 12353-12363.	1.5	7
522	Numerical Simulations of Defective Structures: The Nature of Oxygen Vacancy in Non-reducible (MgO,) Tj ETQq0 0 0 rgBT /Overlock 10 T	0.3	7

#	Article	IF	Citations
523	Ferromagnetism in nitrogen-doped BaO: a self-interaction corrected DFT study. Physical Chemistry Chemical Physics, 2017, 19, 3279-3286.	1.3	7
524	Influence of Strain on Acidâ€“Basic Properties of Oxide Surfaces. Journal of Physical Chemistry C, 2020, 124, 19126-19135.	1.5	7
525	Structure and Band Alignment of InP Photocatalysts Passivated by TiO₂ Thin Films. Journal of Physical Chemistry C, 2021, 125, 11620-11627.	1.5	7
526	Pseudopotential calculations on hydrogen bonded systems : H2O, CH3OH and HCOOH dimers. Molecular Physics, 1979, 38, 1865-1874.	0.8	6
527	The electronic structure of small metallic clusters. Part II. Pseudopotential calculations of lithium clusters, Lin, of increasing nuclearity (8 â©½ n â©½ 32). Journal of Molecular Catalysis, 1981, 12, 213-220.	1.2	6
528	Zero-bias conductance anomaly of a FeO-bound Au atom triggered by CO adsorption. Physical Review B, 2009, 79, .	1.1	6
529	Mechanism of the Cycloâ€Oligomerisation of C₂H₂ on Anatase TiO₂ (101) and (001) Surfaces and Their Reduction: An Electron Paramagnetic Resonance and Density Functional Theory Study. ChemPlusChem, 2016, 81, 64-72.	1.3	6
530	Precursor chemistry of h-BN: adsorption, desorption, and decomposition of borazine on Pt(110). Physical Chemistry Chemical Physics, 2020, 22, 11704-11712.	1.3	6
531	Role of support in tuning the properties of single atom catalysts: Cu, Ag, Au, Ni, Pd, and Pt adsorption on SiO2/Ru, SiO2/Pt, and SiO2/Si ultrathin films. Journal of Chemical Physics, 2021, 154, 134706.	1.2	6
532	Continuous network structure of two-dimensional silica across a supporting metal step edge: An atomic scale study. Physical Review Materials, 2021, 5, .	0.9	6
533	Size and Shape Dependence of the Electronic Structure of Gold Nanoclusters on TiO2. Journal of Physical Chemistry Letters, 2021, 12, 8363-8369.	2.1	6
534	AB INITIO THEORY OF POINT DEFECTS IN SiO2. , 2000, , 161-195.		6
535	Density Functional Cluster Calculations on Metal Deposition at Oxide Surfaces. , 1997, , 353-370.		6
536	Prediction of 2D ferromagnetism and monovalent europium ions in EuBr/graphene heterojunctions. Physical Chemistry Chemical Physics, 2021, 23, 25500-25506.	1.3	6
537	First principles approach to solar energy conversion efficiency of semiconductor heterojunctions. Solar Energy, 2022, 236, 445-454.	2.9	6
538	Molecular orbital study of the bridging dioxygen ligand in [Al2(CH3)6(O2)]?. Journal of the Chemical Society Dalton Transactions, 1987, , 355.	1.1	5
539	Surface electronic structure of heavily-ion-implanted and laser-annealed Si single crystals. Physical Review B, 1990, 41, 3728-3732.	1.1	5
540	The electronic structure of an oxygen defect in NiO (100). Chemical Physics Letters, 1994, 219, 107-112.	1.2	5

#	Article	IF	Citations
541	Vibrations of CO on strained Cu(100) surfaces. A cluster model analysis. Chemical Physics Letters, 1996, 259, 438-444.	1.2	5
542	Vibrational frequencies of CO adsorbed on silica supported Mo atoms from density functional calculations. Journal of Molecular Catalysis A, 2001, 170, 175-186.	4.8	5
543	Theory of Nanoscale Atomic Lithography. An ab Initio Study of the Interaction of â€œcoldâ€•Cs Atoms with Organthiols Self-assembled Monolayers on Au(111). Journal of Physical Chemistry B, 2005, 109, 1815-1821.	1.2	5
544	g-tensor and hyperfine splitting of {m Cl}_{2}^{-} , {m O}_{2}^{-} , {m N}_{2}^{-} defect centers in KCl from DFT calculations. Modelling and Simulation in Materials Science and Engineering, 2009, 17, 084005.	0.8	5
545	Nb-doped CaO: an efficient electron donor system. Journal of Physics Condensed Matter, 2014, 26, 315004.	0.7	5
546	Characterization of Oâ˜-Centers on Single Crystalline MgO(001)-Films. Topics in Catalysis, 2015, 58, 811-823.	1.3	5
547	Ferromagnetic Interactions in Highly Stable, Partially Reduced TiO₂: The S=2 State in Anatase. Angewandte Chemie, 2017, 129, 2648-2651.	1.6	5
548	Chemical Reactivity of Supported ZnO Clusters: Undercoordinated Zinc and Oxygen Atoms as Active Sites. ChemPhysChem, 2020, 21, 2553-2564.	1.0	5
549	Interface Oxygen Induced Internal Structures of Ultrathin MgO Islands Grown on Ag(100). Journal of Physical Chemistry C, 2020, 124, 8834-8842.	1.5	5
550	Iso-valent doping of reducible oxides: a comparison of rutile (110) and anatase (101) TiO₂ surfaces. Journal of Physics Condensed Matter, 2021, 33, 494001.	0.7	5
551	Magnetic nature and hyperfine interactions of transition metal atoms adsorbed on ultrathin insulating films: a challenge for DFT. Physical Chemistry Chemical Physics, 2022, 24, 15891-15903.	1.3	5
552	The electronic structure of small metallic clusters Part V: A SCF î—¸ CI calculation of the interaction of molecular hydrogen with a Li4 cluster. Journal of Molecular Catalysis, 1981, 13, 379-388.	1.2	4
553	Size-dependent dissociation of small cobalt clusters on ultrathin NaCl films. Nano Research, 2017, 10, 1832-1839.	5.8	4
554	Growth and characterization of Caâ€”Mo mixed oxide films on Mo(001). Journal of Chemical Physics, 2019, 151, 234708.	1.2	4
555	Assessing the film-substrate interaction in germania films on reconstructed Au(111). Physical Review B, 2019, 100, .	1.1	4
556	A DFT study of formic acid decomposition on the stoichiometric SnO2 surface as a function of iso-valent doping. Surface Science, 2022, 718, 122009.	0.8	4
557	Role of Structural Flexibility on the Physical and Chemical Properties of Metal-Supported Oxide Ultrathin Films. Springer Series in Materials Science, 2016, , 91-118.	0.4	3
558	Modelling of an ultra-thin silicatene/silicon-carbide hybrid film. Journal of Physics Condensed Matter, 2016, 28, 364005.	0.7	3

#	Article	IF	Citations
559	CH3Br adsorption on MgO/Mo ultrathin films: A DFT study. Surface Science, 2018, 672-673, 1-6.	0.8	3
560	Excited States in Metal Oxides by Configuration Interaction and Multireference Perturbation Theory. Progress in Theoretical Chemistry and Physics, 2000, , 227-245.	0.2	3
561	Some comments on the stable forms of small alkali metal clusters. Journal of Physics B: Atomic and Molecular Physics, 1986, 19, L451-L454.	1.6	2
562	Pseudopotential multireference single and double excited configuration interaction calculations of nickel-containing molecules. 4. HNiSiH3 and HNiAlH3 as minimum models of hydrogen atoms chemisorption on a supported nickel atom. The Journal of Physical Chemistry, 1991, 95, 4795-4800.	2.9	2
563	Role of Point Defects in the Catalytic Activation of Pd Atoms Supported on the MgO Surface. Progress in Theoretical Chemistry and Physics, 2001, , 183-198.	0.2	2
564	Comparativeab initiostudy of the structure and stability ofHâ^'andLiâ^'anions in silica networks. Physical Review B, 2004, 69, .	1.1	2
565	Theory of Metal Clusters on the MgO Surface: The Role of Point Defects. Nanoscience and Technology, 2007, , 193-243.	1.5	2
566	Structure and dynamics of CaO films: A computational study of an effect of external static electric field. Physical Review B, 2017, 95, .	1.1	2
567	From Crystalline to Amorphous Germania Bilayer Films at the Atomic Scale: Preparation and Characterization. Angewandte Chemie, 2019, 131, 11019-11024.	1.6	2
568	Structural and electronic properties of TiO2 from first principles calculations. , 2021, , 67-85.		2
569	Ionic Bonding of Adsorbates on Surfaces: Theoretical Characterization and Observable Consequences. NATO ASI Series Series B: Physics, 1992, , 233-250.	0.2	2
570	Structure and Properties of Metal Clusters and Colloids in Ligand Shells. , 1996, , 355-370.		2
571	Growth of Nâ€Heterocyclic Carbene Assemblies on Cu(100) and Cu(111): from Single Molecules to Magicâ€Number Islands. Angewandte Chemie, 0, , .	1.6	2
572	Defect engineering of oxide surfaces: dream or reality?. Journal of Physics Condensed Matter, 2022, 34, 291501.	0.7	2
573	Computer generation of symmetry-adapted molecular orbitals. Computers & Chemistry, 1981, 5, 111-115.	1.2	1
574	Bonding in nickel cluster carbonyls. Zeitschrift FÃ¼r Physik D-Atoms Molecules and Clusters, 1989, 12, 395-397.	1.0	1
575	Coordination of dihydrogen to transition metal complexes: ab initio investigation of Cr(CO)5(H2) and Cr(CO)4(H2)2. Journal of Organometallic Chemistry, 1989, 377, C13-C16.	0.8	1
576	Surfaces are different: A perspective on structural, energetic and electronic properties of (001) surfaces of alkaline earth metal oxides as calculated with hybrid density functional theory by Andrew J. Logsdail, David Mora-Fonz, David O. Scanlon, C. Richard A. Catlow, Alexey A. Sokol. Surface Science, 2015, 642, 66-67.	0.8	1

#	Article	IF	Citations
577	Structures and properties of Pd nanoparticles intercalated in layered TiO2: A computational study. Catalysis Today, 2021, , .	2.2	1
578	Quantum Chemistry of Chemisorption at Metal and Oxide Surfaces: A Cluster Model Approach. , 1993, , 317-340.		1
579	SIMULATIONS OF UV INDUCED PROCESSES IN SILICA GLASSES. , 2001, , .		1
580	Theoretical Investigation of Surface Relaxation Effects on Chemisorption of Atomic Oxygen on Aluminum Clusters. , 1987, , 843-848.		1
581	From Li clusters to nanocatalysis: A brief tour of 40Åyears of cluster chemistry. Inorganica Chimica Acta, 2022, 530, 120680.	1.2	1
582	Pseudopotential MRD CI calculations of nickel-containing molecules. III. NiSiH3 and NiAlH3 as minimum models of metal-support systems. Chemical Physics, 1990, 142, 369-380.	0.9	0
583	H-H bond activation in transition metal complexes: An MO-LCAO study of the ligands effect. Rendiconti Lincei, 1991, 2, 221-226.	1.0	0
584	Physisorbed and chemisorbed CO2 at surface and step sites of the MgO(100) surface. Surface Science Letters, 1993, 281, 174.	0.1	0
585	The Ground and Excited States of Oxides. , 2002, , 93-109.		0
586	Alkali Metal Doping of MgO: Mechanisms of Formation of Paramagnetic Surface Centers. ChemInform, 2003, 34, no.	0.1	0
587	Post Hartree-Fock and Density Functional Theory Formalisms. , 2006, , 185-215.		0
588	Metal Nanoparticles on Oxide Ultrathin Films: A Class of Materials with Unprecedented Properties. ECS Meeting Abstracts, 2009, , .	0.0	0
589	Reprint of â€œTheoretical description of metal/oxide interfacial properties: The case of MgO/Ag(001)â€• Applied Surface Science, 2017, 396, 1850-1854.	3.1	0
590	Frontispiece: Growth and Atomicâ€Scale Characterization of Ultrathin Silica and Germania Films: The Crucial Role of the Metal Support. Chemistry - A European Journal, 2021, 27, .	1.7	0
591	Frontispiece: Rational Design of Semiconductor Heterojunctions for Photocatalysis. Chemistry - A European Journal, 2021, 27, .	1.7	0
592	Abâ€“initio simulations of photo-induced interconversions of oxygen deficient centers in amorphous silica. , 2001, , .		0
593	Electronic Structure and Chemisorption Properties of Supported Metal Clusters. , 2003, , .		0
594	Cluster Model Calculations of the Interaction of H and CO with Small Pd Clusters. , 1986, , 465-475.		0

#	Article	IF	Citations
595	Molecular Metal Clusters: Structures and Bonding. Springer Series in Materials Science, 1988, , 364-376.	0.4	0
596	Bonding in nickel cluster carbonyls. , 1989, , 395-397.		0