Francesc Illas Riera

List of Publications by Year
in descending order

665	30,984	4955 84	11601 135
papers	citations	h-index	g-index

695	695	695	22086
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	Support nanostructure boosts oxygen transfer to catalytically active platinum nanoparticles. Nature Materials, 2011, 10, 310-315.	13.3	748
2	A New Type of Strong Metalâ€“Support Interaction and the Production of H₂ through the Transformation of Water on Pt/CeO₂(111) and Pt/CeO_x/TiO₂(110) Catalysts. Journal of the American Chemical Society, 2012, 134, 8968-8974.	6.6	682
3	First-principlesLDA+UandGGA+Ustudy of cerium oxides: Dependence on the effective U parameter. Physical Review B, 2007, 75, .	1.1	634
4	Origin of the Large N 1s Binding Energy in X-ray Photoelectron Spectra of Calcined Carbonaceous Materials. Journal of the American Chemical Society, 1996, 118, 8071-8076.	6.6	490
5	A Molecular Mechanism for the Chemoselective Hydrogenation of Substituted Nitroaromatics with Nanoparticles of Gold on TiO₂ Catalysts:â€‰ A Cooperative Effect between Gold and the Support. Journal of the American Chemical Society, 2007, 129, 16230-16237.	6.6	458
6	Remarks on the Proper Use of the Broken Symmetry Approach to Magnetic Coupling. Journal of Physical Chemistry A, 1997, 101, 7860-7866.	1.1	421
7	Maximum Nobleâ€Metal Efficiency in Catalytic Materials: Atomically Dispersed Surface Platinum. Angewandte Chemie - International Edition, 2014, 53, 10525-10530.	7.2	384
8	Effect of Fock exchange on the electronic structure and magnetic coupling in NiO. Physical Review B, 2002, 65, .	1.1	360
9	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
10	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
11	Magnetic coupling in biradicals, binuclear complexes and wide-gap insulators: a survey of ab initio wave function and density functional theory approaches. Theoretical Chemistry Accounts, 2000, 104, 265-272.	0.5	268
12	Antiferromagnetic Exchange Interactions from Hybrid Density Functional Theory. Physical Review Letters, 1997, 79, 1539-1542.	2.9	264
13	Bulk Properties of Transition Metals: A Challenge for the Design of Universal Density Functionals. Journal of Chemical Theory and Computation, 2014, 10, 3832-3839.	2.3	245
14	MXenes: New Horizons in Catalysis. ACS Catalysis, 2020, 10, 13487-13503.	5.5	239
15	CO2 hydrogenation on Au/TiC, Cu/TiC, and Ni/TiC catalysts: Production of CO, methanol, and methane. Journal of Catalysis, 2013, 307, 162-169.	3.1	214
16	Performance of the M06 family of exchange-correlation functionals for predicting magnetic coupling in organic and inorganic molecules. Journal of Chemical Physics, 2008, 128, 114103.	1.2	208
17	Decomposition of the chemisorption bond by constrained variations: Order of the variations and construction of the variational spaces. Journal of Chemical Physics, 1992, 96, 8962-8970.	1.2	205
18	A unified view of the theoretical description of magnetic coupling in molecular chemistry and solid state physics. Physical Chemistry Chemical Physics, 2006, 8, 1645.	1.3	200

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19	Dramatic reduction of the oxygen vacancy formation energy in ceria particles: a possible key to their remarkable reactivity at the nanoscale. Journal of Materials Chemistry, 2010, 20, 10535.	6.7	192
20	Atomic and electronic structure of molybdenum carbide phases: bulk and low Miller-index surfaces. Physical Chemistry Chemical Physics, 2013, 15, 12617.	1.3	189
21	Establishing the Accuracy of Broadly Used Density Functionals in Describing Bulk Properties of Transition Metals. Journal of Chemical Theory and Computation, 2013, 9, 1631-1640.	2.3	184
22	A systematic density functional theory study of the electronic structure of bulk and (001) surface of transition-metals carbides. Journal of Chemical Physics, 2005, 122, 174709.	1.2	180
23	The bending machine: CO₂ activation and hydrogenation on Î´-MoC(001) and Î²-Mo₂C(001) surfaces. Physical Chemistry Chemical Physics, 2014, 16, 14912-14921.	1.3	175
24	An Empirical, yet Practical Way To Predict the Band Gap in Solids by Using Density Functional Band Structure Calculations. Journal of Physical Chemistry C, 2017, 121, 18862-18866.	1.5	165
25	Greatly facilitated oxygen vacancy formation in ceria nanocrystallites. Chemical Communications, 2010, 46, 5936.	2.2	160
26	First Principles Analysis of the Stability and Diffusion of Oxygen Vacancies in Metal Oxides. Physical Review Letters, 2004, 93, 225502.	2.9	158
27	Graphene on Ni(111): Coexistence of Different Surface Structures. Journal of Physical Chemistry Letters, 2011, 2, 759-764.	2.1	158
28	Ab Initio Modeling of the Metalâ^'Support Interface:Â The Interaction of Ni, Pd, and Pt on MgO(100). Journal of Physical Chemistry B, 1998, 102, 1430-1436.	1.2	156
29	Understanding the reactivity of metallic nanoparticles: beyond the extended surface model for catalysis. Chemical Society Reviews, 2014, 43, 4922-4939.	18.7	156
30	Transition metal carbides as novel materials for CO₂ capture, storage, and activation. Energy and Environmental Science, 2016, 9, 141-144.	15.6	155
31	First-principles calculations of the atomic and electronic structure ofFcenters in the bulk and on the (001) surface ofSrTiO3. Physical Review B, 2006, 73, .	1.1	152
32	CO₂abatement using two-dimensional MXene carbides. Journal of Materials Chemistry A, 2018, 6, 3381-3385.	5.2	152
33	On the activation of molecular hydrogen by gold: a theoretical approximation to the nature of potential active sites. Chemical Communications, 2007, , 3371.	2.2	146
34	Transition metal adatoms on graphene: A systematic density functional study. Carbon, 2015, 95, 525-534.	5.4	144
35	Active Sites for H₂Adsorption and Activation in Au/TiO₂and the Role of the Support. Journal of Physical Chemistry A, 2009, 113, 3750-3757.	1.1	142
36	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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37	Highly Active Au/Î´-MoC and Cu/Î´-MoC Catalysts for the Conversion of CO₂: The Metal/C Ratio as a Key Factor Defining Activity, Selectivity, and Stability. Journal of the American Chemical Society, 2016, 138, 8269-8278.	6.6	140
38	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
39	Accounting for van der Waals interactions between adsorbates and surfaces in density functional theory based calculations: selected examples. RSC Advances, 2013, 3, 13085.	1.7	138
40	Low-Basicity Oxygen Atoms: A Key in the Search for Propylene Epoxidation Catalysts. Angewandte Chemie - International Edition, 2007, 46, 2055-2058.	7.2	134
41	Bonding Mechanisms of Graphene on Metal Surfaces. Journal of Physical Chemistry C, 2012, 116, 7360-7366.	1.5	133
42	Magnetic coupling in ionic solids studied by density functional theory. Journal of Chemical Physics, 1998, 108, 2519-2527.	1.2	131
43	Multiconfigurational Perturbation Theory:Â An Efficient Tool to Predict Magnetic Coupling Parameters in Biradicals, Molecular Complexes, and Ionic Insulators. Journal of Physical Chemistry A, 2001, 105, 11371-11378.	1.1	129
44	CO₂ Activation and Methanol Synthesis on Novel Au/TiC and Cu/TiC Catalysts. Journal of Physical Chemistry Letters, 2012, 3, 2275-2280.	2.1	129
45	Methane Activation by Platinum: Critical Role of Edge and Corner Sites of Metal Nanoparticles. Chemistry - A European Journal, 2010, 16, 6530-6539.	1.7	126
46	Density functional studies of model cerium oxide nanoparticles. Physical Chemistry Chemical Physics, 2008, 10, 5730.	1.3	125
47	Why Copper Is Intrinsically More Selective than Silver in Alkene Epoxidation:Â Ethylene Oxidation on Cu(111) versus Ag(111). Journal of the American Chemical Society, 2005, 127, 10774-10775.	6.6	124
48	Extent and limitations of density-functional theory in describing magnetic systems. Physical Review B, 2004, 70, .	1.1	122
49	On the Promoting Role of Ag in Selective Hydrogenation Reactions over Pdâ^'Ag Bimetallic Catalysts:â€‰ A Theoretical Study. Journal of Physical Chemistry C, 2007, 111, 6852-6856.	1.5	121
50	Ultralow-Density Nanocage-Based Metal-Oxide Polymorphs. Physical Review Letters, 2007, 99, 235502.	2.9	119
51	Theoretical analysis of the bonding of oxygen to Cu(100). Physical Review B, 1990, 42, 10852-10857.	1.1	118
52	Local character of magnetic coupling in ionic solids. Physical Review B, 1999, 59, R6593-R6596.	1.1	117
53	Electronic structure of a neutral oxygen vacancy inSrTiO3. Physical Review B, 2003, 68, .	1.1	116
54	Restricted Ensemble-Referenced Kohnâ^'Sham versus Broken Symmetry Approaches in Density Functional Theory:â€‰ Magnetic Coupling in Cu Binuclear Complexes. Journal of Chemical Theory and Computation, 2007, 3, 764-774.	2.3	113

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55	Accurate Prediction of Large Antiferromagnetic Interactions in High-TcHgBa2Canâ^'1CunO2n+2+Î´(n=2,3) Superconductor Parent Compounds. Physical Review Letters, 2000, 84, 1579-1582.	2.9	111
56	Mechanism of selective alcohol oxidation to aldehydes on gold catalysts: Influence of surface roughness on reactivity. Journal of Catalysis, 2011, 278, 50-58.	3.1	110
57	Critical Size for O₂ Dissociation by Au Nanoparticles. ChemPhysChem, 2009, 10, 348-351.	1.0	108
58	Density Functional Theory Study of the Interaction of Cu, Ag, and Au Atoms with the Regular CeO₂(111) Surface. Journal of Physical Chemistry C, 2010, 114, 1934-1941.	1.5	108
59	Effective and Highly Selective CO Generation from CO₂ Using a Polycrystalline Î±-Mo₂C Catalyst. ACS Catalysis, 2017, 7, 4323-4335.	5.5	108
60	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
61	Discrepancy between common local aromaticity measures in a series of carbazole derivatives. Physical Chemistry Chemical Physics, 2004, 6, 314-318.	1.3	106
62	Comparative study of the molecular electrostatic potential obtained from different wavefunctions. Reliability of the semiempirical MNDO wavefunction. Journal of Computational Chemistry, 1990, 11, 416-430.	1.5	105
63	Measures of ionicity of alkaline-earth oxides from the analysis ofab initiocluster wave functions. Physical Review B, 1993, 48, 11573-11582.	1.1	105
64	Approaching nanoscale oxides: models and theoretical methods. Chemical Society Reviews, 2009, 38, 2657.	18.7	105
65	Ab Initio Study of the Exchange Coupling in Oxalato-Bridged Cu(II) Dinuclear Complexes. Journal of Physical Chemistry A, 2000, 104, 9983-9989.	1.1	103
66	Ab initio theoretical comparative study of magnetic coupling inKNiF3sandK2NiF4s. Physical Review B, 1997, 55, 4129-4137.	1.1	102
67	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
68	The conversion of CO₂ to methanol on orthorhombic Î²-Mo₂C and Cu/Î²-Mo₂C catalysts: mechanism for admetal induced change in the selectivity and activity. Catalysis Science and Technology, 2016, 6, 6766-6777.	2.1	101
69	Comment on â€œAbout the calculation of exchange coupling constants using density-functional theory: The role of the self-interaction errorâ€•[J. Chem. Phys. 123, 164110 (2005)]. Journal of Chemical Physics, 2006, 124, 107101.	1.2	99
70	Understanding Ceria Nanoparticles from First-Principles Calculations. Journal of Physical Chemistry C, 2007, 111, 10142-10145.	1.5	99
71	On modelling the interaction of CO on the MgO(100) surface. Surface Science, 1995, 327, 59-73.	0.8	96
72	Influence of step sites in the molecular mechanism of the water gas shift reaction catalyzed by copper. Journal of Catalysis, 2009, 268, 131-141.	3.1	96

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73	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
74	MXenes as promising catalysts for water dissociation. Applied Catalysis B: Environmental, 2020, 260, 118191.	10.8	94
75	A Systematic Study of the Structure and Bonding of Halogens on Low-Index Transition Metal Surfaces. Journal of Physical Chemistry B, 2006, 110, 11894-11906.	1.2	93
76	Nature of Ag Islands and Nanoparticles on the CeO₂(111) Surface. Journal of Physical Chemistry C, 2012, 116, 1122-1132.	1.5	92
77	Good performance of the M06 family of hybrid meta generalized gradient approximation density functionals on a difficult case: CO adsorption on MgO(001). Journal of Chemical Physics, 2008, 129, 124710.	1.2	90
78	Validation of Koopmans' theorem for density functional theory binding energies. Physical Chemistry Chemical Physics, 2015, 17, 4015-4019.	1.3	90
79	Effects of deposited Pt particles on the reducibility of CeO2(111). Physical Chemistry Chemical Physics, 2011, 13, 11384.	1.3	89
80	Activation of noble metals on metal-carbide surfaces: novel catalysts for CO oxidation, desulfurization and hydrogenation reactions. Physical Chemistry Chemical Physics, 2012, 14, 427-438.	1.3	89
81	Role of Auâ^'C Interactions on the Catalytic Activity of Au Nanoparticles Supported on TiC(001) toward Molecular Oxygen Dissociation. Journal of the American Chemical Society, 2010, 132, 3177-3186.	6.6	88
82	When Anatase Nanoparticles Become Bulklike: Properties of Realistic TiO₂ Nanoparticles in the 1â€“6 nm Size Range from All Electron Relativistic Density Functional Theory Based Calculations. Journal of Chemical Theory and Computation, 2017, 13, 1785-1793.	2.3	87
83	Descriptors controlling the catalytic activity of metallic surfaces toward water splitting. Journal of Catalysis, 2010, 276, 92-100.	3.1	86
84	Importance of Madelung potential in quantum chemical modeling of ionic surfaces. Journal of Computational Chemistry, 1997, 18, 617-628.	1.5	85
85	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
86	Structure and Properties of Zirconia Nanoparticles from Density Functional Theory Calculations. Journal of Physical Chemistry C, 2016, 120, 4392-4402.	1.5	85
87	Theoretical study of bulk and surface oxygen and aluminum vacancies inÎ±â^'Al2O3. Physical Review B, 2004, 69, .	1.1	84
88	Effect of the exchange-correlation potential and of surface relaxation on the description of the H2O dissociation on Cu(111). Journal of Chemical Physics, 2009, 130, 224702.	1.2	84
89	Electronic and magnetic structure of bulk cobalt: The Î±, Î², and Îµ-phases from density functional theory calculations. Journal of Chemical Physics, 2010, 133, 024701.	1.2	83
90	Reactivity of Transition Metals (Pd, Pt, Cu, Ag, Au) toward Molecular Hydrogen Dissociation: Extended Surfaces versus Particles Supported on TiC(001) or Small Is Not Always Better and Large Is Not Always Bad. Journal of Physical Chemistry C, 2011, 115, 11666-11672.	1.5	82

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91	When Langmuir Is Too Simple:H2Dissociation on Pd(111) at High Coverage. Physical Review Letters, 2004, 93, 146103.	2.9	81
92	Catalyst size matters: Tuning the molecular mechanism of the waterâ€“gas shift reaction on titanium carbide based compounds. Journal of Catalysis, 2008, 260, 103-112.	3.1	81
93	Functionalization of Î³-graphyne by transition metal adatoms. Carbon, 2017, 120, 63-70.	5.4	81
94	Bandgap Engineering of Graphene by Physisorbed Adsorbates. Advanced Materials, 2011, 23, 2638-2643.	11.1	80
95	Theoretical Approaches to Excited-State-Related Phenomena in Oxide Surfaces. Chemical Reviews, 2013, 113, 4456-4495.	23.0	80
96	Predicting size-dependent emergence of crystallinity in nanomaterials: titania nanoclusters versus nanocrystals. Nanoscale, 2017, 9, 1049-1058.	2.8	79
97	Ab Initio Cluster Model Study of the Chemisorption of CO on Low-Index Platinum Surfaces. Journal of Physical Chemistry B, 1999, 103, 5246-5255.	1.2	78
98	Theoretical Confirmation of the Enhanced Facility to Increase Oxygen Vacancy Concentration in TiO₂by Iron Doping. Journal of Physical Chemistry C, 2010, 114, 6511-6517.	1.5	78
99	Spin Symmetry Requirements in Density Functional Theory: The Proper Way to Predict Magnetic Coupling Constants in Molecules and Solids. Theoretical Chemistry Accounts, 2006, 116, 587-597.	0.5	77
100	Effect of electron correlation on the electrostatic potential distribution of molecules. Journal of the American Chemical Society, 1991, 113, 5203-5211.	6.6	76
101	Quantum-Chemical Study of Electrochemical Promotion in Catalysis. The Journal of Physical Chemistry, 1996, 100, 16653-16661.	2.9	76
102	Evidence for spontaneous CO2 activation on cobalt surfaces. Chemical Physics Letters, 2008, 454, 262-268.	1.2	76
103	Rigorous characterization of oxygen vacancies in ionic oxides. Physical Review B, 2002, 66, .	1.1	75
104	Size-Dependent Level Alignment between Rutile and Anatase TiO₂ Nanoparticles: Implications for Photocatalysis. Journal of Physical Chemistry Letters, 2017, 8, 5593-5598.	2.1	75
105	Madelung fields from optimized point charges forab initiocluster model calculations on ionic systems. Journal of Computational Chemistry, 1993, 14, 680-684.	1.5	74
106	Interaction of CO and NO with PdCu(111) Surfaces. Journal of Physical Chemistry B, 1998, 102, 8017-8023.	1.2	74
107	Reliability of range-separated hybrid functionals for describing magnetic coupling in molecular systems. Journal of Chemical Physics, 2008, 129, 184110.	1.2	74
108	Edge sites as a gate for subsurface carbon in palladium nanoparticles. Journal of Catalysis, 2009, 266, 59-63.	3.1	71

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109	Adsorption, Oxidation State, and Diffusion of Pt Atoms on the CeO₂(111) Surface. Journal of Physical Chemistry C, 2010, 114, 14202-14207.	1.5	71
110	A Semiempirical Method to Detect and Correct DFT-Based Gas-Phase Errors and Its Application in Electrocatalysis. ACS Catalysis, 2020, 10, 6900-6907.	5.5	71
111	Selected versus complete configuration interaction expansions. Journal of Chemical Physics, 1991, 95, 1877-1883.	1.2	70
112	Desulfurization of Thiophene on Au/TiC(001): Auâ^'C Interactions and Charge Polarization. Journal of the American Chemical Society, 2009, 131, 8595-8602.	6.6	70
113	Prediction of core level binding energies in density functional theory: Rigorous definition of initial and final state contributions and implications on the physical meaning of Kohn-Sham energies. Journal of Chemical Physics, 2015, 142, 214102.	1.2	70
114	Towards anab initiodescription of magnetism in ionic solids. Physical Review Letters, 1993, 71, 3549-3552.	2.9	69
115	H2Cracking at SiO2Defect Centersâ€. Journal of Physical Chemistry A, 2000, 104, 4674-4684.	1.1	69
116	Dissociation of SO₂ on Au/TiC(001): Effects of Auâ€“C Interactions and Charge Polarization. Angewandte Chemie - International Edition, 2008, 47, 6685-6689.	7.2	69
117	Critical effect of carbon vacancies on the reverse water gas shift reaction over vanadium carbide catalysts. Applied Catalysis B: Environmental, 2020, 267, 118719.	10.8	69
118	Electronic Structure of F-Doped Bulk Rutile, Anatase, and Brookite Polymorphs of TiO₂. Journal of Physical Chemistry C, 2012, 116, 12738-12746.	1.5	68
119	BrÃ¸nstedâ€“Evansâ€“Polanyi Relationship for Transition Metal Carbide and Transition Metal Oxide Surfaces. Journal of Physical Chemistry C, 2013, 117, 4168-4171.	1.5	67
120	Charge Polarization at a Auâ€“TiC Interface and the Generation of Highly Active and Selective Catalysts for the Lowâ€Temperature Waterâ€“Gas Shift Reaction. Angewandte Chemie - International Edition, 2014, 53, 11270-11274.	7.2	67
121	Facile Heterogeneously Catalyzed Nitrogen Fixation by MXenes. ACS Catalysis, 2020, 10, 5049-5056.	5.5	67
122	Chemisorption of atomic chlorine on metal surfaces and the interpretation of the induced work function changes. Surface Science, 2005, 574, 297-305.	0.8	66
123	Density Functional Study of the Adsorption of Atomic Oxygen on the (001) Surface of Early Transition-Metal Carbides. Journal of Physical Chemistry C, 2007, 111, 1307-1314.	1.5	66
124	Adsorption of gold on TiC(001): Auâ€“C interactions and charge polarization. Journal of Chemical Physics, 2007, 127, 211102.	1.2	66
125	On the interaction of polycyclic aromatic compounds with graphene. Carbon, 2012, 50, 2482-2492.	5.4	66
126	Origin of the vibrational shift of CO chemisorbed on Pt(111). Physical Review B, 1995, 52, 12372-12379.	1.1	65

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127	Theoretical aspects of heterogeneous catalysis: Applications of density functional methods. Catalysis Today, 2005, 105, 2-16.	2.2	65
128	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
129	On the difficulties of present theoretical models to predict the oxidation state of atomic Au adsorbed on regular sites of CeO[sub 2](111). Journal of Chemical Physics, 2009, 131, 094702.	1.2	64
130	Fundamentals of Methanol Synthesis on Metal Carbide Based Catalysts: Activation of CO2 and H2. Topics in Catalysis, 2015, 58, 159-173.	1.3	64
131	Challenges of modeling nanostructured materials for photocatalytic water splitting. Chemical Society Reviews, 2022, 51, 3794-3818.	18.7	64
132	Can corundum be described as an ionic oxide?. Journal of Chemical Physics, 1993, 99, 6818-6823.	1.2	62
133	Dynamic Ion Pairs in the Adsorption of Isolated Water Molecules on Alkaline-Earth Oxide (001) Surfaces. Physical Review Letters, 2008, 100, 016101.	2.9	62
134	Origin of magnetic coupling inLa2CuO4. Physical Review B, 1996, 53, 945-951.	1.1	61
135	On the bonding mechanism of CO to Pt(111) and its effect on the vibrational frequency of chemisorbed CO. Surface Science, 1997, 376, 279-296.	0.8	61
136	Bulk and surface oxygen vacancy formation and diffusion in single crystals, ultrathin films, and metal grown oxide structures. Journal of Chemical Physics, 2006, 125, 074711.	1.2	61
137	Density functional studies of coinage metal nanoparticles: scalability of their properties to bulk. Theoretical Chemistry Accounts, 2008, 120, 565-573.	0.5	61
138	SO₂ Adsorption on Pt(111) and Oxygen Precovered Pt(111): A Combined Infrared Reflection Absorption Spectroscopy and Density Functional Study. Journal of Physical Chemistry C, 2011, 115, 479-491.	1.5	61
139	Formation of One-Dimensional Electronic States along the Step Edges of CeO₂(111). ACS Nano, 2012, 6, 1126-1133.	7.3	61
140	Inexpensive determinations of valence virtual MOs for CI calculations. Chemical Physics, 1986, 107, 361-380.	0.9	60
141	Ab initiostudy of the magnetic interactions in the spin-ladder compoundSrCu2O3. Physical Review B, 1999, 60, 3457-3464.	1.1	60
142	A Systematic Density Functional Study of Molecular Oxygen Adsorption and Dissociation on the (001) Surface of Group IVâ^'VI Transition Metal Carbides. Journal of Physical Chemistry C, 2007, 111, 16982-16989.	1.5	60
143	Systematic study of the effect of HSE functional internal parameters on the electronic structure and band gap of a representative set of metal oxides. Journal of Computational Chemistry, 2017, 38, 781-789.	1.5	60
144	Jacobâ€™s Ladder as Sketched by Escher: Assessing the Performance of Broadly Used Density Functionals on Transition Metal Surface Properties. Journal of Chemical Theory and Computation, 2018, 14, 395-403.	2.3	60

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145	Evidence for oxygen-island formation on Al(111): Cluster-model theory and x-ray photoelectron spectroscopy. Physical Review B, 1991, 44, 9025-9034.	1.1	59
146	Ionic-covalent transition in titanium oxides. Physical Review B, 1994, 50, 13974-13980.	1.1	59
147	Designing water splitting catalysts using rules of thumb: advantages, dangers and alternatives. Physical Chemistry Chemical Physics, 2020, 22, 6797-6803.	1.3	59
148	Relative Stabilities of Low Index and Stepped CeO₂ Surfaces from Hybrid and GGA + U Implementations of Density Functional Theory. Journal of Physical Chemistry C, 2011, 115, 3716-3721.	1.5	58
149	Theoretical assessment of graphene-metal contacts. Journal of Chemical Physics, 2013, 138, 244701.	1.2	58
150	Electric field effects in heterogeneous catalysis. Journal of Molecular Catalysis A, 1997, 119, 263-273.	4.8	57
151	Magnetic structure ofLi2CuO2:â€ƒFromab initiocalculations to macroscopic simulations. Physical Review B, 2002, 66, .	1.1	57
152	Room Temperature Methane Capture and Activation by Ni Clusters Supported on TiC(001): Effects of Metalâ€“Carbide Interactions on the Cleavage of the Câ€“H Bond. Journal of the American Chemical Society, 2019, 141, 5303-5313.	6.6	57
153	Electronic structure and magnetic interactions of the spin-chain compoundsCa2CuO3andSr2CuO3. Physical Review B, 2000, 63, .	1.1	56
154	Three Lanthanum MOF Polymorphs: Insights into Kinetically and Thermodynamically Controlled Phases. Inorganic Chemistry, 2009, 48, 4707-4713.	1.9	56
155	Density functional theory model study of size and structure effects on water dissociation by platinum nanoparticles. Journal of Chemical Physics, 2012, 137, 034701.	1.2	56
156	The Tripletâ€“Singlet Gap in the m-Xylylene Radical: A Not So Simple One. Journal of Chemical Theory and Computation, 2014, 10, 335-345.	2.3	56
157	Study of the Heterometallic Bond Nature in PdCu(111) Surfaces. Journal of Physical Chemistry B, 1998, 102, 141-147.	1.2	55
158	Two-dimensional nitrides as highly efficient potential candidates for CO₂ capture and activation. Physical Chemistry Chemical Physics, 2018, 20, 17117-17124.	1.3	55
159	Thickness biased capture of CO₂ on carbide MXenes. Physical Chemistry Chemical Physics, 2019, 21, 23136-23142.	1.3	55
160	The structural relaxation of the Î±-Al2O3(0001) â€“ an investigation of potential errors. Chemical Physics Letters, 2001, 341, 412-418.	1.2	54
161	Density Functional Theory Study of the Adsorption of Au Atom on Cerium Oxide: Effect of Low-Coordinated Surface Sites. Journal of Physical Chemistry C, 2009, 113, 4948-4954.	1.5	54
162	Affordable Estimation of Solvation Contributions to the Adsorption Energies of Oxygenates on Metal Nanoparticles. Journal of Physical Chemistry C, 2019, 123, 5578-5582.	1.5	54

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163	Treating large intermediate spaces in the CIPSI method through a direct selected CI algorithm. Theoretica Chimica Acta, 1992, 82, 229-238.	0.9	53
164	On the Mechanism of Formation of Metal Nanowires by Selfâ€Assembly. Angewandte Chemie - International Edition, 2007, 46, 7094-7097.	7.2	53
165	Effect of Size and Structure on the Ground-State and Excited-State Electronic Structure of TiO₂ Nanoparticles. Journal of Chemical Theory and Computation, 2016, 12, 3751-3763.	2.3	53
166	Kinetic Monte Carlo simulations of the water gas shift reaction on Cu(1 1 1) from density functional theory based calculations. Journal of Catalysis, 2016, 333, 217-226.	3.1	53
167	Assessing GW Approaches for Predicting Core Level Binding Energies. Journal of Chemical Theory and Computation, 2018, 14, 877-883.	2.3	53
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