Javier FernÃ¡ndez Sanz

List of Publications by Year
in descending order

206 papers	8,915 citations	43973 48 h-index	49773 87 g-index
216 all docs	216 docs citations	216 times ranked	9761 citing authors

#	Article	IF	Citations
1	Highly active copper-ceria and copper-ceria-titania catalysts for methanol synthesis from CO ₂. Science, 2014, 345, 546-550.	6.0	1,114
2	Importance of the Metalâ€“Oxide Interface in Catalysis: In Situ Studies of the Waterâ€“Gas Shift Reaction by Ambientâ€Pressure Xâ€ray Photoelectron Spectroscopy. Angewandte Chemie - International Edition, 2013, 52, 5101-5105.	7.2	280
3	Waterâ€Gas Shift Reaction on a Highly Active Inverse CeO_x/Cu(111) Catalyst: Unique Role of Ceria Nanoparticles. Angewandte Chemie - International Edition, 2009, 48, 8047-8050.	7.2	262
4	High catalytic activity of Au/CeO _x /TiO ₂ (110) controlled by the nature of the mixed-metal oxide at the nanometer level. Proceedings of the National Academy of Sciences of the United States of America, 2009, 106, 4975-4980.	3.3	257
5	Gold, Copper, and Platinum Nanoparticles Dispersed on CeO_x/TiO₂(110) Surfaces: High Water-Gas Shift Activity and the Nature of the Mixed-Metal Oxide at the Nanometer Level. Journal of the American Chemical Society, 2010, 132, 356-363.	6.6	247
6	CO Oxidation on Inverse CeO_x/Cu(111) Catalysts: High Catalytic Activity and Ceria-Promoted Dissociation of O₂. Journal of the American Chemical Society, 2011, 133, 3444-3451.	6.6	241
7	High Waterâ^'Gas Shift Activity in TiO₂(110) Supported Cu and Au Nanoparticles: Role of the Oxide and Metal Particle Size. Journal of Physical Chemistry C, 2009, 113, 7364-7370.	1.5	223
8	Coumarin derivatives for dye sensitized solar cells: a TD-DFT study. Physical Chemistry Chemical Physics, 2012, 14, 225-233.	1.3	193
9	Real-Time TD-DFT Simulations in Dye Sensitized Solar Cells: The Electronic Absorption Spectrum of Alizarin Supported on TiO₂ Nanoclusters. Journal of Chemical Theory and Computation, 2010, 6, 2856-2865.	2.3	170
10	Effect of on-site Coulomb repulsion term<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mi>U</mml:mi></mml:math>on the band-gap states of the reduced rutile (110)<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:mi mathvariant="normal">Ti</mml:mi><mml:msub><mml:mi mathvariant="normal">O</mml:mi><mml:mn>2</mml:mn></mml:msub></mml:mrow></mml:math>surface.	1.1	165
11	Frequency dependent hyperpolarizabilities with application to formaldehyde and methyl fluoride. Journal of Chemical Physics, 1990, 93, 8828-8839.	1.2	132
12	Cu, Ag, and Au atoms adsorbed on TiO2(110): cluster and periodic calculations. Surface Science, 2001, 471, 21-31.	0.8	131
13	Direct vs Indirect Mechanisms for Electron Injection in Dye-Sensitized Solar Cells. Journal of Physical Chemistry C, 2011, 115, 11293-11301.	1.5	129
14	N doping of TiO2(110): Photoemission and density-functional studies. Journal of Chemical Physics, 2006, 125, 094706.	1.2	127
15	Comparative Study on the Performance of Hybrid DFT Functionals in Highly Correlated Oxides: The Case of CeO₂and Ce₂O₃. Journal of Chemical Theory and Computation, 2011, 7, 56-65.	2.3	125
16	Inverse Oxide/Metal Catalysts in Fundamental Studies and Practical Applications: A Perspective of Recent Developments. Journal of Physical Chemistry Letters, 2016, 7, 2627-2639.	2.1	120
17	Au â†” N Synergy and N-Doping of Metal Oxide-Based Photocatalysts. Journal of the American Chemical Society, 2008, 130, 12056-12063.	6.6	115
18	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

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19	N Doping of Rutile TiO₂ (110) Surface. A Theoretical DFT Study. Journal of Physical Chemistry C, 2008, 112, 2624-2631.	1.5	107
20	Methanol Adsorption and Dissociation on TiO2(110) from First Principles Calculations. Journal of Physical Chemistry C, 2007, 111, 10023-10028.	1.5	106
21	Electronic structure and optical spectra of catechol on TiO₂nanoparticles from real time TD-DFT simulations. Physical Chemistry Chemical Physics, 2011, 13, 1506-1514.	1.3	103
22	On modelling the interaction of CO on the MgO(100) surface. Surface Science, 1995, 327, 59-73.	0.8	96
23	A theoretical insight into the catalytic effect of a mixed-metal oxide at the nanometer level: The case of the highly active metal/CeOx/TiO2(110) catalysts. Journal of Chemical Physics, 2010, 132, 104703.	1.2	93
24	Methanol and Water Dissociation on TiO2 (110): The Role of Surface Oxygen. Journal of Physical Chemistry C, 2008, 112, 17737-17740.	1.5	92
25	Graphenes as Efficient Metalâ€Free Fenton Catalysts. Chemistry - A European Journal, 2015, 21, 11966-11971.	1.7	87
26	Accurate ab initio determination of magnetic interactions and hopping integrals in La2â^'xSrxCuO4 systems. Journal of Chemical Physics, 2000, 112, 5158-5167.	1.2	85
27	Electronic charge transfer between ceria surfaces and gold adatoms: a GGA+U investigation. Physical Chemistry Chemical Physics, 2009, 11, 5246.	1.3	83
28	Oxygen vacancies on TiO2 (110) from first principles calculations. Journal of Chemical Physics, 2004, 121, 7427-7433.	1.2	75
29	Electron Mobility via Polaron Hopping in Bulk Ceria: A First-Principles Study. Journal of Physical Chemistry C, 2013, 117, 14502-14509.	1.5	75
30	Nature of the Mixed-Oxide Interface in Ceriaâ€"Titania Catalysts: Clusters, Chains, and Nanoparticles. Journal of Physical Chemistry C, 2013, 117, 14463-14471.	1.5	73
31	First-principles calculations of structural and electronic properties of monoclinic hafnia surfaces. Physical Review B, 2006, 73, .	1.1	71
32	Visible Light-Driven H₂ Production over Highly Dispersed Ruthenia on Rutile TiO₂ Nanorods. ACS Catalysis, 2016, 6, 407-417.	5.5	71
33	Unravelling the Origin of the High-Catalytic Activity of Supported Au:Â A Density-Functional Theory-Based Interpretation. Journal of the American Chemical Society, 2006, 128, 15600-15601.	6.6	65
34	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
35	Cu, Ag and Au atoms deposited on the Î±-Al2O3(0001) surface: a comparative density functional study. Surface Science, 2005, 575, 189-196.	0.8	63
36	Communication: Improving the density functional theory+U description of CeO2 by including the contribution of the O 2p electrons. Journal of Chemical Physics, 2012, 136, 041101.	1.2	62

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37	V@Au12-:Â An Improved Novel Catalyst for CO Oxidation?. Journal of Physical Chemistry B, 2006, 110, 11600-11603.	1.2	61
38	Molecular-dynamics simulations of liquid aluminum oxide. Physical Review B, 1998, 58, 2369-2371.	1.1	60
39	Theoretical Investigation of the Deposition of Cu, Ag, and Au Atoms on the ZrO2(111) Surface. Journal of Physical Chemistry C, 2007, 111, 10448-10454.	1.5	58
40	Interaction of Pd withÎ±â^'Al2O3(0001):â€ƒA case study of modeling the metal-oxide interface on complex substrates. Physical Review B, 2002, 65, .	1.1	55
41	Surface model and exchange-correlation functional effects on the description of Pd/Î±-Al2O3(0001). Journal of Chemical Physics, 2002, 116, 1684-1691.	1.2	51
42	Interaction of oxygen with TiN(001):Nâ†"O exchange and oxidation process. Journal of Chemical Physics, 2007, 126, 244713.	1.2	51
43	Adsorption of Pd Atoms and Dimers on the TiO2(110) Surface:â€‰ A First Principles Study. Journal of Physical Chemistry C, 2007, 111, 3949-3955.	1.5	51
44	Molecular dynamics studies of the structure of Î³-alumina. Chemical Physics Letters, 1992, 192, 463-468.	1.2	50
45	Role of vacancies in the structural stability ofÎ±â^'TiO: A first-principles study based on density-functional calculations. Physical Review B, 2005, 72, .	1.1	50
46	Sonogashira Cross-Coupling and Homocoupling on a Silver Surface: Chlorobenzene and Phenylacetylene on Ag(100). Journal of the American Chemical Society, 2015, 137, 940-947.	6.6	50
47	Computer Simulation of .gamma.-Al2O3 Microcrystal. The Journal of Physical Chemistry, 1995, 99, 17872-17876.	2.9	49
48	Direct vs. indirect mechanisms for electron injection in DSSC: Catechol and alizarin. Computational and Theoretical Chemistry, 2011, 975, 99-105.	1.1	49
49	Effect of dispersion correction on the Au(1 1 1)-H2O interface: A first-principles study. Journal of Chemical Physics, 2012, 137, 114709.	1.2	49
50	Changing the physical and chemical properties of titanium oxynitrides<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:mrow><mml:msub><mml:mrow><mml:mtext>TiN</mml:mtext></mml:mrow><mml:mrow><mml:mn>1</mml:m changing the composition. Physical Review B, 2009, 80, .	1.1	48
51	Determining the Behavior of RuO_x Nanoparticles in Mixedâ€Metal Oxides: Structural and Catalytic Properties of RuO₂/TiO₂(110) Surfaces. Angewandte Chemie - International Edition, 2011, 50, 10198-10202.	7.2	48
52	Ab initio systematic determination of the tâ€"J effective Hamiltonian parameters for superconducting Cu-oxides. Chemical Physics Letters, 1999, 307, 102-108.	1.2	47
53	Electronic structure of the transition-metal-carbene-like complexes (CO)5Mo-M'H2 (M' = carbon,) Tj ETQq1 1 0.784314 rgBT /Overloc American Chemical Society, 1992, 114, 2903-2909.	6.6	46
54	Molecular-dynamics simulations of(NaO2)x(SiO2)1â^'xglasses: Relation between distribution and diffusive behavior of Na atoms. Physical Review B, 1998, 58, 9047-9053.	1.1	46

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55	Atomic Layer Deposition of Hafnium Oxide from Hafnium Chloride and Water. Journal of the American Chemical Society, 2008, 130, 11996-12006.	6.6	45
56	Surface models for Î³-Al2O3from molecular dynamics simulations. Journal of the Chemical Society, Faraday Transactions, 1993, 89, 3623-3628.	1.7	44
57	Drifts, XPS, XAS, and ab Initio Study of Lanthanide Oxides Supported on .gamma.-Al2O3. The Journal of Physical Chemistry, 1995, 99, 4655-4660.	2.9	44
58	Cu Deposited on CeOx-Modified TiO₂(110): Synergistic Effects at the Metalâ€“Oxide Interface and the Mechanism of the WGS Reaction. ACS Catalysis, 2016, 6, 4608-4615.	5.5	43
59	Surface structure of cubic aluminum oxide. Physical Review B, 1994, 50, 2561-2565.	1.1	41
60	Transport Properties in the CeO_{2â€“x}(111) Surface: From Charge Distribution to Ion-Electron Collaborative Migration. Journal of Physical Chemistry C, 2013, 117, 25497-25503.	1.5	41
61	Compact model potentials for ab initio embedded cluster calculations. Part I. Basic formulation. Journal of Chemical Physics, 1995, 102, 327-336.	1.2	40
62	Carbon Doping of the TiO₂ (110) Rutile Surface. A Theoretical Study Based on DFT. Chemistry of Materials, 2009, 21, 1431-1438.	3.2	39
63	Theoretical calculations of proton affinities of azines. Prediction of the relative basicities and preferred protonation sites. Journal of Computational Chemistry, 1988, 9, 784-789.	1.5	38
64	N2O Decomposition on TiO2 (110) from Dynamic First-Principles Calculations. Journal of Physical Chemistry B, 2005, 109, 16223-16226.	1.2	38
65	Nitrogen/gold codoping of the TiO2(101) anatase surface. A theoretical study based on DFT calculations. Physical Chemistry Chemical Physics, 2011, 13, 11340.	1.3	38
66	Waterâ€“Gas Shift Reaction on K/Cu(111) and Cu/K/TiO₂(110) Surfaces: Alkali Promotion of Water Dissociation and Production of H₂. ACS Catalysis, 2019, 9, 10751-10760.	5.5	38
67	Molecular dynamics simulations of Na deposition on the TiO2(110) surface. Surface Science, 1998, 409, 92-100.	0.8	37
68	Synthesis, Solid-State Structure, and Bonding Analysis of the Beryllocenes[Be(C5Me4H)2],[Be(C5Me5)2], and[Be(C5Me5)(C5Me4H)]. Chemistry - A European Journal, 2003, 9, 4452-4461.	1.7	37
69	Mechanism of Cu Deposition on theÎ±â^'Al2O3(0001) Surface. Physical Review Letters, 2005, 94, 016104.	2.9	37
70	Molecular modification of coumarin dyes for more efficient dye sensitized solar cells. Journal of Chemical Physics, 2012, 136, 194702.	1.2	36
71	Structural, electronic and optical properties of copper, silver and gold sulfide: a DFT study. Theoretical Chemistry Accounts, 2016, 135, 1.	0.5	35
72	First Principles Study of Cu Atoms Deposited on the Î±-Al2O3(0001) Surface. Journal of Physical Chemistry B, 2002, 106, 11495-11500.	1.2	34

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73	Structural Defects in W-Doped TiO₂ (101) Anatase Surface: Density Functional Study. Journal of Physical Chemistry C, 2011, 115, 16970-16976.	1.5	34
74	Direct determination of the effective electronic coupling in electron-transfer problems. The Journal of Physical Chemistry, 1993, 97, 99-106.	2.9	33
75	Spectroscopic properties and potential energy curves of some low-lying electronic states of AlO, AlO+, LaO, and LaO+: An ab initioCASSCFstudy. International Journal of Quantum Chemistry, 1994, 52, 1329-1338.	1.0	33
76	Unraveling the Nature of the Oxideâ€“Metal Interaction in Ceria-Based Noble Metal Inverse Catalysts. Journal of Physical Chemistry C, 2014, 118, 26931-26938.	1.5	33
77	The Flexible Surface Revisited: Adsorbate-Induced Reconstruction, Homocoupling, and Sonogashira Cross-Coupling on the Au(100) Surface. Journal of Physical Chemistry C, 2014, 118, 11677-11684.	1.5	31
78	Molecular Dynamics Simulations of Pd Deposition on the Î±-Al2O3(0001) Surface. Journal of Physical Chemistry B, 2001, 105, 12111-12117.	1.2	30
79	Density Functional Theory Study of Co, Rh, and Ir Atoms Deposited on the Î±-Al2O3(0001) Surface. Journal of Physical Chemistry B, 2004, 108, 15671-15678.	1.2	30
80	First-Principles Investigation of Hydroxylated Monoclinic HfO2 Surfaces. Chemistry of Materials, 2006, 18, 3397-3403.	3.2	30
81	Thiodiacetateâ€“Manganese Chemistry with N ligands: Unique Control of the Supramolecular Arrangement over the Metal Coordination Mode. Chemistry - A European Journal, 2011, 17, 10600-10617.	1.7	29
82	Making Photo-selective TiO₂ Materials by Cationâ€“Anion Codoping: From Structure and Electronic Properties to Photoactivity. Journal of Physical Chemistry C, 2012, 116, 18759-18767.	1.5	29
83	Designing a new generation of catalysts: Water gas shift reaction example. Catalysis Today, 2015, 240, 214-219.	2.2	29
84	Supramolecular Interactions as Determining Factors of the Geometry of Metallic Building Blocks: Tetracarboxylate Dimanganese Species. Angewandte Chemie - International Edition, 2005, 44, 3429-3432.	7.2	27
85	Simulating the optical properties of CdSe clusters using the RT-TDDFT approach. Theoretical Chemistry Accounts, 2013, 132, 1.	0.5	27
86	Gold Nanoparticles on Yttrium Modified Titania: Support Properties and Catalytic Activity. Topics in Catalysis, 2011, 54, 219-228.	1.3	25
87	Adsorption of Acetone onto MgO: Experimental and Theoretical Evidence for the Presence of a Surface Enolate. Angewandte Chemie - International Edition, 1999, 38, 506-509.	7.2	24
88	Molecular Dynamics Simulations of the Structure of Pd Clusters Deposited on the MgO(001) Surface. Journal of Physical Chemistry B, 2000, 104, 4342-4348.	1.2	24
89	Role of Coverage and Surface Oxidation Degree in the Adsorption of Acetone on TiO₂(110). A Density Functional Study. Journal of Physical Chemistry C, 2009, 113, 19973-19980.	1.5	24
90	Surface oxygen vacancies in gold based catalysts for CO oxidation. RSC Advances, 2014, 4, 13145-13152.	1.7	24

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91	Adsorption of Pd atoms on Î³-Al2O3: a density functional study of metalâ€“support interactions. Applied Surface Science, 2004, 238, 82-85.	3.1	23
92	Solvent effects on the dissociation of aliphatic carboxylic acids in waterâ€” N,N -dimethylformamide mixtures. Analytica Chimica Acta, 1990, 228, 301-306.	2.6	22
93	The vacuum-ultraviolet spectrum of iron pentacarbonyl: An experimental analysis supported by a CASSCF CCI study of the Rydberg states. The Journal of Physical Chemistry, 1992, 96, 121-123.	2.9	22
94	Reactions of {[Pd(Î¼-SC6F5)(Î¼-dppm)Pd](Î¼-SC6F5)}4Â·2O(C2H5)2. Crystal Structures of the Complexes [(Ph3P)Pd(Î¼-SC6F5)(Î¼-dppm)Pd(SC6F5)]Â·1.4CH2Cl2and [(Ph3P)Pd(Î¼-SC6F5)(Î¼-dppm)Pd(PPh3)]SO3CF3Â·2CH2Cl2andabInitioMO Calculations on the Model Systems [(H3P)Pd(Î¼-H2PCH2PH2)(Î¼-SH)Pd(PH3)]+and [(H3P)Pd(Î¼-H2PCH2PH2)Pd(PH3)]2+. Inorganic Chemistry, 1997, 36, 1912-1922.	1.9	22
95	Theoretical Analysis of K Adsorption on TiO2(110) Rutile Surface. Journal of Physical Chemistry B, 1999, 103, 480-486.	1.2	22
96	Understanding Acetaldehyde Thermal Chemistry on the TiO₂ (110) Rutile Surface: From Adsorption to Reactivity. Journal of Physical Chemistry C, 2011, 115, 2819-2825.	1.5	22
97	Comprehensive Experimental and Theoretical Study of the CO + NO Reaction Catalyzed by Au/Ni Nanoparticles. ACS Catalysis, 2019, 9, 4919-4929.	5.5	22
98	Charting the Lattice Thermal Conductivities of Iâ€“IIIâ€“VI₂ Chalcopyrite Semiconductors. Chemistry of Materials, 2022, 34, 2833-2841.	3.2	22
99	Physical Factors Governing the Amplitude of the Electron Transfer Integral in Mixed-Valence Compounds. Journal of Physical Chemistry A, 1998, 102, 3659-3667.	1.1	21
100	Adsorption of Prototypical Asphaltenes on Silica: First-Principles DFT Simulations Including Dispersion Corrections. Journal of Physical Chemistry B, 2018, 122, 618-624.	1.2	21
101	Ab initio CASSCF study of the electronic structure of the transition-metal alkylidene-like complexes Mo-M'H2 (M' = carbon, silicon, germanium and tin). Journal of the American Chemical Society, 1992, 114, 10019-10024.	6.6	20
102	Theoretical models for ?-Al2O3 (110) surface hydroxylation: An ab initio embedded cluster study. International Journal of Quantum Chemistry, 1998, 70, 359-365.	1.0	20
103	Dedicated Molecular Orbitals for the Variational Determination of the Electron-Transfer Matrix Element. Method and Application to a Cu(I)â^'Cu(II) Mixed Valence Compound. Journal of Physical Chemistry A, 1997, 101, 1716-1721.	1.1	19
104	First principles study of Na adsorption on TiO2 (110) surface. International Journal of Quantum Chemistry, 1998, 70, 351-357.	1.0	19
105	First principles simulations of Cu and Au deposition on Î±-Al2O3 (0001) surface. Applied Surface Science, 2004, 238, 228-232.	3.1	19
106	Graphene Translucency and Interfacial Interactions in the Gold/Graphene/SiC System. Journal of Physical Chemistry Letters, 2018, 9, 3850-3855.	2.1	19
107	Ab initio CI calculations on the molecular structure of Sn2H4 isomers. Chemical Physics, 1989, 138, 99-104.	0.9	18
108	Geometric and Electronic Structure of Amorphous Aluminophosphates. Ab Initio and Experimental Studies. Journal of Physical Chemistry B, 1997, 101, 9510-9516.	1.2	18

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109	A periodic Hartreeâ€“Fock study of Na adsorption on the TiO2(110) rutile surface. Chemical Physics Letters, 1999, 303, 111-116.	1.2	18
110	Ab Initio Calculations of the Electron-Transfer Matrix Element in Culâ¯CuIIMixed-Valence Compounds. Journal of the American Chemical Society, 1998, 120, 1051-1061.	6.6	17
111	Synthesis, Structural Characterization, and MO Calculations of Vanadium Imido Complexes Containing Bidentate Phosphine Coligands. Inorganic Chemistry, 1999, 38, 4462-4466.	1.9	17
112	Charge state of metal atoms on oxide supports: a systematic study based on simulated infrared spectroscopy and density functional theory. Theoretical Chemistry Accounts, 2010, 126, 265-273.	0.5	17
113	First-principles molecular dynamics simulations of the H2O / Cu(111) interface. Journal of Molecular Modeling, 2012, 18, 2433-2442.	0.8	17
114	Ag₂S Quantum Dot-Sensitized Solar Cells by First Principles: The Effect of Capping Ligands and Linkers. Journal of Physical Chemistry A, 2017, 121, 7290-7296.	1.1	17
115	Molecular dynamics simulations of the MgO(001) surface hydroxylation. Journal of Chemical Physics, 1998, 108, 4219-4225.	1.2	16
116	Understanding the Interplay of Dopants, Interfaces, and Anionic Conductivity in Doped Ceria/Zirconia Heteroepitaxial Structures. Chemistry of Materials, 2014, 26, 3385-3390.	3.2	16
117	Effect of Capping Ligands and TiO₂ Supporting on the Optical Properties of a (CdSe)₁₃ Cluster. Journal of Physical Chemistry A, 2015, 119, 1218-1227.	1.1	16
118	Molecular dynamics simulations of the role of salinity and temperature on the hydrocarbon/water interfacial tension. Theoretical Chemistry Accounts, 2017, 136, 1.	0.5	16
119	AM1 study of the protonation of pteridine-related tetraazanaphthalenes. Journal of Organic Chemistry, 1988, 53, 3900-3903.	1.7	15
120	Reactivity of diazoazoles with electron-rich double bonds. Journal of the Chemical Society Perkin Transactions II, 1990, , 1943-1950.	0.9	15
121	Abinitiogroup model potentials: Application to the study of intermolecular interactions. Journal of Chemical Physics, 1993, 99, 1255-1261.	1.2	15
122	Parallel computation of second derivatives of RHF energy on distributed memory computers. Journal of Computational Chemistry, 1997, 18, 159-168.	1.5	15
123	Relaxation of the surface in binary Sc, Ti and V nitrides: a first principles density functional study. Surface Science, 2003, 541, 217-224.	0.8	15
124	Onset of perovskite formation in the catalytic system La2O3/?-Al2O3. Catalysis Letters, 1993, 21, 89-97.	1.4	14
125	Ab Initio SCF-Mo Study of the Chemisorption of Methane on Al and La Oxide Surfaces. Journal of Catalysis, 1995, 156, 273-278.	3.1	14
126	Unrestricted compact model potentials for ab initio embedded cluster calculations: Magnetic interactions in KNiF3. Journal of Chemical Physics, 1995, 102, 850-858.	1.2	14

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127	Potassium and Water Coadsorption on TiO₂(110): OH-Induced Anchoring of Potassium and the Generation of Single-Site Catalysts. Journal of Physical Chemistry Letters, 2016, 7, 3866-3872.	2.1	14
128	Cr2O3 (0001) oxygen-terminating surface. A molecular dynamics study. Computational and Theoretical Chemistry, 1999, 463, 185-190.	1.5	13
129	A method for including environment polarization effects in ab initio cluster embedded calculations. Application to the water deprotonation over an ideal Alî—¸MgO surface. Chemical Physics, 1995, 191, 133-139.	0.9	12
130	The thermostabilising effect of La doping on Î³-Al2O3 a molecular dynamics simulation study. Solid State Ionics, 1997, 95, 73-79.	1.3	12
131	Ab initio study of the adsorption of acetone and keto-enol equilibrium on the MgO(100) surface. Surface Science, 1998, 397, 23-33.	0.8	12
132	DFTversus CI determination of the electron-transfer matrix element in some case examples. International Journal of Quantum Chemistry, 2000, 76, 458-463.	1.0	12
133	Theoretical Approach to Ionic Conductivity in PhosphorusOxynitride Compounds. Journal of Solid State Chemistry, 2001, 161, 73-79.	1.4	12
134	A Density Functional Study of Initial Steps in the Oxidation of Early Transition Metal Nitrides, MN (M =) Tj ETQq0 0 0 rgBT /Overlock 10 T	1.5	12
135	Redox properties of gold-substituted zirconia surfaces. Journal of Materials Chemistry, 2009, 19, 710-717.	6.7	12
136	Effects of the capping ligands, linkers and oxide surface on the electron injection mechanism of copper sulfide quantum dot-sensitized solar cells. Physical Chemistry Chemical Physics, 2017, 19, 14580-14587.	1.3	12
137	Photo-sensitizing thin-film ferroelectric oxides using materials databases and high-throughput calculations. Journal of Materials Chemistry A, 2019, 7, 27323-27333.	5.2	12
138	Ab initio calculations of molecular and electronic structure of disilane. I. Molecular force field and vibrational spectrum. Chemical Physics, 1991, 149, 311-318.	0.9	11
139	Evaluation of solvent effects on the dissociation of aliphatic carboxylic acids in aqueousN,N-dimethylformamide mixtures according to the scaled particle theory. Journal of Physical Organic Chemistry, 1991, 4, 87-95.	0.9	11
140	A theoretical study of the Naî—¸TiO2 (001) rutile interaction. Journal of Molecular Catalysis A, 1997, 119, 135-142.	4.8	11
141	A first principles study of Pd deposition on the TiO 2 (1 1 0) surface. Theoretical Chemistry Accounts, 2000, 104, 317-322.	0.5	11
142	Influence of Temperature on the Interaction between Pd Clusters and the<mml:math xmlns:mml="http://www.w3.org/1998/Math/MathML" display="inline"><mml:msub><mml:mi>TiO</mml:mi><mml:mn>2</mml:mn></mml:msub></mml:math>(110) Surface. Physical Review Letters, 2007, 99, 066102.	2.9	11
143	First-Principles Investigation of the Structure, Energetics, and Electronic Properties of Ru/HfO2Interfaces. Journal of Physical Chemistry C, 2007, 111, 9203-9210.	1.5	11
144	Molecular-dynamics simulations of premelting processes inCr2O3. Physical Review B, 1998, 58, 6057-6062.	1.1	10

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145	MO Rationalization of the Synthesis and Structure of V(N-2,6-iPr2C6H3)Cl(CO)2(PMe3)2 Complex. Organometallics, 2000, 19, 304-308.	1.1	10
146	Coverage and charge dependent adsorption of butanethiol on the Au(111) surface: A density functional theory study. Computational and Theoretical Chemistry, 2011, 975, 116-121.	1.1	10
147	Adsorption of prototypical amino acids on silica: Influence of the pre-adsorbed water multilayer. Surface Science, 2016, 646, 239-246.	0.8	10
148	Micropore formation mechanisms in Î³Al2O3. Surface Science, 1995, 322, 185-192.	0.8	9
149	A Theoretical Study of ZnCH2 and ZnSnH2 Electronic Structure and the ZnCH2â^'HZnCH Photolytic Rearrangement. Journal of the American Chemical Society, 1996, 118, 429-436.	6.6	9
150	Experimental and molecular dynamics simulation analysis of LaCrO3 precipitation in chromia scales. Acta Materialia, 2000, 48, 2951-2958.	3.8	9
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