Monica Calatayud

List of Publications by Year
in descending order

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112 papers	4,236 citations	76294 40 h-index	128225 60 g-index
117 all docs	117 docs citations	117 times ranked	5057 citing authors

#	Article	IF	Citations
1	Understanding the Role of Oxygen Vacancies in the Water Gas Shift Reaction on Ceria-Supported Platinum Catalysts. ACS Catalysis, 2014, 4, 2088-2096.	5.5	176
2	Adsorption on perfect and reduced surfaces of metal oxides. Catalysis Today, 2003, 85, 125-143.	2.2	142
3	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
4	Diffusion versus Desorption: Complex Behavior of H Atoms on an Oxide Surface. ChemPhysChem, 2008, 9, 253-256.	1.0	127
5	Static simulation of bulk and selected surfaces of anatase TiO2. Surface Science, 2001, 490, 116-124.	0.8	115
6	Comparison of the reduction of metal oxide surfaces: TiO2-anatase, TiO2-rutile and SnO2-rutile. Surface Science, 2005, 583, 107-117.	0.8	110
7	A Systematic Density Functional Theory Study of VxOy+ and VxOY (X = 2â^'4, Y = 2â^'10) Systems. Journal of Physical Chemistry A, 2001, 105, 9760-9775.	1.1	107
8	Periodic study on the structural and electronic properties of bulk, oxidized and reduced SnO 2 (1 1 0) surfaces and the interaction with O 2. Surface Science, 2002, 511, 408-420.	0.8	100
9	Periodic DFT Study of the Structural and Electronic Properties of Bulk CoAl2O4Spinel. Journal of Physical Chemistry B, 2006, 110, 988-995.	1.2	80
10	Predicting size-dependent emergence of crystallinity in nanomaterials: titania nanoclusters versus nanocrystals. Nanoscale, 2017, 9, 1049-1058.	2.8	79
11	Modeling catalytic reduction of NO by ammonia over V2O5. Surface Science Reports, 2004, 55, 169-236.	3.8	75
12	Characterization of Supported Vanadium Oxide Species on Silica: A Periodic DFT Investigation. Journal of Physical Chemistry C, 2009, 113, 10740-10746.	1.5	75
13	Effect of relaxation on structure and reactivity of anatase (100) and (001) surfaces. Surface Science, 2004, 552, 169-179.	0.8	73
14	A theoretical study on the structure, energetics and bonding of VOx+ and VOx (x=1â€“4) systems. Chemical Physics Letters, 2001, 333, 493-503.	1.2	72
15	A theoretical analysis of adsorption and dissociation of CH3OH on the stoichiometric SnO2(110) surface. Surface Science, 1999, 430, 213-222.	0.8	70
16	Theoretical Investigation of the Hydrogenation of (TiO₂)_NClusters (N= 1â€“10). Journal of Physical Chemistry C, 2011, 115, 15890-15899.	1.5	69
17	Quantum-mechanical analysis of the equation of state of anataseTiO2. Physical Review B, 2001, 64, .	1.1	68
18	Theoretical Study on the Molecular Mechanism for the Reaction of VO2+ with C2H4. Journal of Physical Chemistry A, 2003, 107, 3107-3120.	1.1	68

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19	Stability of Hydroxylated (1Ì„11) and (1Ì„01) Surfaces of Monoclinic Zirconia:â€‰ A Combined Study by DFT and Infrared Spectroscopy. Journal of Physical Chemistry C, 2008, 112, 6469-6476.	1.5	68
20	Scaling reducibility of metal oxides. Theoretical Chemistry Accounts, 2017, 136, 1.	0.5	67
21	Reactivity of (TiO₂)_N Clusters (N = 1â^'10): Probing Gas-Phase Acidity and Basicity Properties. Journal of Physical Chemistry C, 2008, 112, 16087-16095.	1.5	66
22	Promoted ceria catalysts for alkyne semi-hydrogenation. Journal of Catalysis, 2015, 324, 69-78.	3.1	65
23	The hierarchy of localization basins: a tool for the understanding of chemical bonding exemplified by the analysis of the VO x and VO x + (x =1-4) systems. Theoretical Chemistry Accounts, 2001, 105, 299-308.	0.5	64
24	Characterization of amorphous silica based catalysts using DFT computational methods. Catalysis Today, 2020, 354, 3-18.	2.2	63
25	Structure and Stability of Formates and Carbonates on Monoclinic Zirconia: A Combined Study by Density Functional Theory and Infrared Spectroscopy. Journal of Physical Chemistry C, 2008, 112, 16096-16102.	1.5	62
26	Theoretical Study on the Role of Surface Basicity and Lewis Acidity on the Etherification of Glycerol over Alkaline Earth Metal Oxides. Chemistry - A European Journal, 2009, 15, 10864-10870.	1.7	62
27	Stability of formate species on Î²-Ga2O3. Physical Chemistry Chemical Physics, 2009, 11, 1397.	1.3	58
28	Revealing the Surface Reactivity of Zirconia by Periodic DFT Calculations. Journal of Physical Chemistry C, 2012, 116, 6636-6644.	1.5	58
29	A periodic model for the V2O5â€“TiO2 (anatase) catalyst. Stability of dimeric species. Surface Science, 2003, 526, 297-308.	0.8	56
30	Direct Evidence of Chelated Geometry of Catechol on TiO₂ by a Combined Solid-State NMR and DFT Study. Journal of Physical Chemistry C, 2016, 120, 23625-23630.	1.5	55
31	Lithium insertion and mobility in the TiO2-anatase/titanate structure: A periodic DFT study. Journal of Electroanalytical Chemistry, 2005, 581, 216-223.	1.9	52
32	Proton ordered cubic and hexagonal periodic models of ordinary ice. Chemical Physics Letters, 2005, 409, 110-117.	1.2	50
33	Electron-count control on adsorption upon reducible and irreducible clean metal-oxide surfaces. Catalysis Today, 2004, 89, 269-278.	2.2	49
34	Effect of Alkali Doping on a V2O5/TiO2Catalyst from Periodic DFT Calculations. Journal of Physical Chemistry C, 2007, 111, 6411-6417.	1.5	49
35	CO oxidation over anatase TiO2-(001). Computational and Theoretical Chemistry, 2004, 709, 73-78.	1.5	47
36	Reactivity of gas-phase, crystal and supported V2O5 systems studied using density functional theory based reactivity indices. Chemical Physics Letters, 2008, 456, 59-63.	1.2	47

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37	Dopamine Adsorption on TiO₂ Anatase Surfaces. Journal of Physical Chemistry C, 2014, 118, 20688-20693.	1.5	47
38	Breaking H₂ with CeO₂: Effect of Surface Termination. ACS Omega, 2018, 3, 16063-16073.	1.6	47
39	Migration of the subsurfaceCimpurity inPd(111). Physical Review B, 2005, 71, .	1.1	43
40	What do vanadium framework sites look like in redox model silicate zeolites?. Microporous and Mesoporous Materials, 2009, 119, 137-143.	2.2	43
41	Ionic interactions: Comparative topological approach. Computational and Theoretical Chemistry, 2012, 998, 193-201.	1.1	41
42	Reactivity of the Oxygen Sites in the V2O5/TiO2Anatase Catalyst. Journal of Physical Chemistry B, 2004, 108, 15679-15685.	1.2	40
43	Combining theoretical description with experimental in situ studies on the effect of alkali additives on the structure and reactivity of vanadium oxide supported catalysts. Catalysis Today, 2008, 139, 209-213.	2.2	39
44	Is There a Nanosize for the Activity of TiO₂ Compounds?. Journal of Physical Chemistry C, 2009, 113, 12186-12194.	1.5	37
45	Theoretical study of ZnO (1010) and Cu/ZnO (1010) surfaces. Chemical Physics Letters, 2001, 338, 224-230.	1.2	35
46	Reactivity of the V2O5â€“TiO2-anatase catalyst: role of the oxygen sites. Topics in Catalysis, 2006, 41, 17-26.	1.3	35
47	Surface Reduction Mechanism of Ceriumâ€“Gallium Mixed Oxides with Enhanced Redox Properties. Journal of Physical Chemistry C, 2013, 117, 8822-8831.	1.5	33
48	Existence and Properties of Isolated Catalytic Sites on the Surface of Î²-Cristobalite-Supported, Doped Tungsten Oxide Catalysts (WO_x/Î²-SiO₂,) Tj ETQq0 0 0 rgBT /Overlock 10 Tf 50 307 Td (Na-WO<sub> Oxidative Coupling of Methane (OCM): A Combined Periodic DFT and Experimental Study. ACS Catalysis, 2020, 10, 4580-4592.	5.5	33
49	Ionization of HCl and HF in ice: a periodic DFT study. Chemical Physics Letters, 2003, 369, 287-292.	1.2	32
50	Stability of Binary SAMs Formed by ï‰-Acid and Alcohol Functionalized Thiol Mixtures. Langmuir, 2009, 25, 9980-9985.	1.6	32
51	Periodic DFT Study of Rutile IrO₂: Surface Reactivity and Catechol Adsorption. Journal of Physical Chemistry C, 2017, 121, 13135-13143.	1.5	32
52	Insights on hydride formation over cerium-gallium mixed oxides: A mechanistic study for efficient H2 dissociation. Journal of Catalysis, 2017, 345, 258-269.	3.1	32
53	Hydrogen Adsorption on Monoclinic (1Ì…11) and (1Ì…01) ZrO₂ Surfaces: A Periodic ab Initio Study. Journal of Physical Chemistry C, 2010, 114, 11918-11923.	1.5	31
54	Photoactivity of Moleculeâ€“TiO₂ Clusters with Time-Dependent Density-Functional Theory. Journal of Physical Chemistry A, 2016, 120, 5115-5124.	1.1	30

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55	Combining theoretical description with experimental in situ studies on the effect of potassium on the structure and reactivity of titania-supported vanadium oxide catalyst. Catalysis Today, 2007, 126, 96-102.	2.2	29
56	Dynamics of Hydration in Vanadiaâ€“Titania Catalysts at Low Loading: A Theoretical and Experimental Study. Journal of Physical Chemistry C, 2011, 115, 24133-24142.	1.5	29
57	Controlled selectivity for ethanol steam reforming reaction over doped CeO2 surfaces: The role of gallium. Applied Catalysis B: Environmental, 2020, 277, 119103.	10.8	29
58	A DFT study on the hydrated V2O5-TiO2-anatase catalyst: stability of monomeric species. Theoretical Chemistry Accounts, 2005, 114, 29-37.	0.5	26
59	SERS as a Probe of Charge-Transfer Pathways in Hybrid Dye/Moleculeâ€“Metal Oxide Complexes. Journal of Physical Chemistry C, 2014, 118, 3774-3782.	1.5	25
60	Electron Localization Function and Maximum Probability Domains analysis of semi-ionic oxides crystals, surfaces and surface defects. Computational and Theoretical Chemistry, 2015, 1053, 315-321.	1.1	25
61	Theoretical Investigation of NO Oxidation over TiO2-Anatase. Surface Review and Letters, 2003, 10, 175-182.	0.5	23
62	Correlation between theoretical and experimental investigations of the ammonia adsorption process on the (110)-VSbO4 surface. Catalysis Today, 2010, 158, 178-185.	2.2	23
63	Combined ATR-FTIR and DFT Study of Cyclohexanone Adsorption on Hydrated TiO₂ Anatase Surfaces. Journal of Physical Chemistry C, 2011, 115, 14164-14172.	1.5	23
64	Theoretical and Experimental Study of Light Hydrocarbon Ammoxidation and Oxidative Dehydrogenation on (110)-VSbO₄ Surfaces. Journal of Physical Chemistry C, 2012, 116, 9132-9141.	1.5	23
65	Understanding the Role of Rutile TiO2 Surface Orientation on Molecular Hydrogen Activation. Nanomaterials, 2019, 9, 1199.	1.9	23
66	Theoretical investigation of the inversion parameter in Co3â^'sAlsO4 (s=0â€“3) spinel structures. Solid State Ionics, 2009, 180, 1011-1016.	1.3	22
67	An atom-in-molecules and electron-localization-function study of the interaction between O 2 and V x O y + /V x O y (x = 1, 2, y = 1-5) clusters. Theoretical Chemistry Accounts, 2002, 108, 12-20.	0.5	21
68	Computing the Fukui Function in Solid-State Chemistry: Application to Alkaline Earth Oxides Bulk and Surfaces. Journal of Physical Chemistry A, 2020, 124, 2826-2833.	1.1	20
69	Unraveling the Mechanisms of the Selective Oxidation of Methanol to Formaldehyde in Vanadia Supported on Titania Catalyst. Journal of Physical Chemistry C, 2010, 114, 6039-6046.	1.5	19
70	X-Ray Diffraction and Theoretical Calculationâ€“Supported Formation of Polymorphic Cocrystals Discovered Through Thermal Methods: A Case Study. Journal of Pharmaceutical Sciences, 2019, 108, 3340-3347.	1.6	19
71	A DFT study of methanol dissociation on isolated vanadate groups. Catalysis Today, 2008, 139, 214-220.	2.2	17
72	Comment on â€œImaging of the Hydrogen Subsurface Site in Rutile<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>â€. Physical Review Letters, 2010, 104, 119603; author reply 119604.	2.9	17

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73	Hydration Dynamics for Vanadia/Titania Catalysts at High Loading: A Combined Theoretical and Experimental Study. Journal of Physical Chemistry C, 2013, 117, 25535-25544.	1.5	17
74	Alkali Ion Incorporation into V₂O₅: a Noncovalent Interactions Analysis. Journal of Physical Chemistry C, 2016, 120, 4259-4265.	1.5	17
75	Ethylene glycol interaction on alkaline earth oxides: A periodic DFT study. Catalysis Today, 2010, 152, 88-92.	2.2	16
76	Fano-Liouville Spectral Signatures in Open Quantum Systems. Physical Review Letters, 2015, 115, 113006.	2.9	16
77	Stability of mixed-oxide titanosilicates: dependency on size and composition from nanocluster to bulk. Nanoscale, 2018, 10, 832-842.	2.8	16
78	Cation distributions on CoAl₂O₄and Co₂AlO₄spinels: pressure and temperature effects. High Pressure Research, 2008, 28, 521-524.	0.4	15
79	Unravelling the enhanced reactivity of bulk CeO2 doped with gallium: A periodic DFT study. Chemical Physics Letters, 2012, 519-520, 69-72.	1.2	14
80	Methanol Oxidation to Formaldehyde on VSiBEA Zeolite: A Combined DFT/vdW/Transition Path Sampling and Experimental Study. Journal of Physical Chemistry C, 2015, 119, 13619-13631.	1.5	14
81	Global optimisation of hydroxylated silica clusters: A cascade Monte Carlo Basin Hopping approach. Computational and Theoretical Chemistry, 2017, 1102, 38-43.	1.1	14
82	Spin localization for NO adsorption on surface O atoms of metal oxides. Catalysis Today, 2006, 113, 201-207.	2.2	13
83	Density functional theory study of the oxidation of methanol to formaldehyde on a hydrated vanadia cluster. Journal of Computational Chemistry, 2010, 31, 2493-2501.	1.5	12
84	Toward an Understanding of the Hydrogenation Reaction of MO₂ Gas-Phase Clusters (M =) Tj ETQq0 0 0 rgBT /Overlock 10	1.1	12
85	The role of dispersion forces in metal-supported self-assembled monolayers. Computational and Theoretical Chemistry, 2015, 1053, 322-327.	1.1	12
86	Platinum and platinum based nanoalloys synthesized by wet chemistry. Faraday Discussions, 2015, 181, 19-36.	1.6	11
87	Nonlinear Fano interferences in open quantum systems: An exactly solvable model. Physical Review A, 2016, 93, .	1.0	11
88	The Subsurface Diffusion of Hydrogen on Rutile TiO2 Surfaces: A Periodic DFT Study. Topics in Catalysis, 2022, 65, 270-280.	1.3	11
89	Hydrogen activation on Anatase TiO2: Effect of surface termination. Catalysis Today, 2022, 397-399, 113-120.	2.2	11
90	Theoretical study of H2 dissociation on a ZrO2 cluster. Chemical Physics Letters, 2011, 503, 12-17.	1.2	10

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91	Novel Delta-Ta₂O₅ Structure Obtained from DFT Calculations. Journal of Physical Chemistry C, 2014, 118, 13652-13658.	1.5	10
92	Understanding How in Situ Generated Hydrogen Controls the Morphology of Platinum Nanoparticles. Journal of Physical Chemistry C, 2014, 118, 9290-9298.	1.5	10
93	Properties of hydrated TiO₂ and SiO₂ nanoclusters: dependence on size, temperature and water vapour pressure. Nanoscale, 2018, 10, 21518-21532.	2.8	10
94	H2 Dissociation and Oxygen Vacancy Formation on Ce2O3 Surfaces. Topics in Catalysis, 2019, 62, 956-967.	1.3	9
95	Theoretical analysis of the adsorption of ammoniaâ€“borane and their dehydrogenation products on the (001) surface of TiC and ZrC. Surface Science, 2019, 680, 95-106.	0.8	9
96	Probing Raman Enhancement in a Dopamineâ€“Ti₂O₄ Hybrid Using Stretched Molecular Geometries. Journal of Physical Chemistry A, 2014, 118, 1196-1202.	1.1	8
97	Understanding iridium oxide nanoparticle surface sites by their interaction with catechol. Physical Chemistry Chemical Physics, 2017, 19, 16151-16158.	1.3	8
98	Periodic density functional theory study of maghemite (001) surface. Structure and electronic properties. Surface Science, 2018, 677, 239-253.	0.8	8
99	Butanethiol adsorption and dissociation on Ag (111): A periodic DFT study. Surface Science, 2016, 646, 247-252.	0.8	7
100	Can Supported Reduced Vanadium Oxides form H₂ from CH₃OH? A Computational Gas-Phase Mechanistic Study. Journal of Physical Chemistry A, 2018, 122, 1104-1113.	1.1	7
101	Valenceâ€Shell Electronâ€Pair Repulsion Theory Revisited: An Explanation for Core Polarization. Chemistry - A European Journal, 2019, 25, 10938-10945.	1.7	7
102	Application of dual descriptor to understand the activity of C u/Z r O 2 catalysts in the water gas shift reaction. Journal of Molecular Modeling, 2017, 23, 34.	0.8	6
103	Modelling rutile TiO2nanorod growth preferences: A density functional theory study. Catalysis Today, 2020, 356, 49-55.	2.2	5
104	Restoring the band gap of metal oxide surfaces by redox adsorption. Computational and Theoretical Chemistry, 2004, 709, 87-96.	1.5	4
105	Oxygen Vacancies in Oxide Nanoclusters: When Silica Is More Reducible Than Titania. Frontiers in Chemistry, 2019, 7, 37.	1.8	4
106	Multi-Scale Modelling of Aggregation of TiO2 Nanoparticle Suspensions in Water. Nanomaterials, 2022, 12, 217.	1.9	4
107	Nanoparticle Assembling through Click Chemistry Directed by Mixed SAMs for Magnetic Applications. ACS Applied Nano Materials, 2019, 2, 554-565.	2.4	3
108	Analyzing the TiO₂ surface reactivity based on oxygen vacancies computed by DFT and DFTB methods. Journal of Physics Condensed Matter, 2022, 34, 314004.	0.7	3

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109	On the reductive hydrogenation process of gas-phase metal dioxides: H2 activation or reduction of the metal center, what is more important?. Theoretical Chemistry Accounts, 2019, 138, 1.	0.5	1
110	Adsorption of Electropositive Atoms with an Odd Number of Electrons (H, K, Au) on a Perfect TiO2(110) Surface. , 2009, , .		0
111	Can the environmental TEM confirm atomistic models of adsorbed molecules at surfaces of solids?. Microscopy and Microanalysis, 2019, 25, 1440-1441.	0.2	0
112	Elucidation of the IR of Cu and Mn substituted intraframework SiBEA zeolites. Topics in Catalysis, 0, , 1.	1.3	0