Monica Calatayud

List of Publications by Year in Descending Order

110 papers	3,561 citations	37 h-index	54 g-index
117 ext. papers	3,909 ext. citations	3.9 avg, IF	5.43 L-index

#	Paper	IF	Citations
110	Hydrogen activation on Anatase TiO2: Effect of surface termination. *Catalysis Today*, **2021**,	5.3	3
109	Controlled selectivity for ethanol steam reforming reaction over doped CeO2 surfaces: The role of gallium. *Applied Catalysis B: Environmental*, **2020**, 277, 119103	21.8	10
108	Existence and Properties of Isolated Catalytic Sites on the Surface of β-Cristobalite-Supported, Doped Tungsten Oxide Catalysts (WOx/β-SiO2, Na-WOx/β-SiO2, Mn-WOx/β-SiO2) for Oxidative Coupling of Methane (OCM): A Combined Periodic DFT and Experimental Study. *ACS Catalysis*, **2020**, 10, 4580-4592	13.1	22
107	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	2.8	6
106	Modelling rutile TiO2nanorod growth preferences: A density functional theory study. *Catalysis Today*, **2020**, 356, 49-55	5.3	0
105	Characterization of amorphous silica based catalysts using DFT computational methods. *Catalysis Today*, **2020**, 354, 3-18	5.3	35
104	Can the environmental TEM confirm atomistic models of adsorbed molecules at surfaces of solids?. *Microscopy and Microanalysis*, **2019**, 25, 1440-1441	0.5	
103	Understanding the Role of Rutile TiO Surface Orientation on Molecular Hydrogen Activation. *Nanomaterials*, **2019**, 9,	5.4	12
102	Valence-Shell Electron-Pair Repulsion Theory Revisited: An Explanation for Core Polarization. *Chemistry - A European Journal*, **2019**, 25, 10938-10945	4.8	5
101	H2 Dissociation and Oxygen Vacancy Formation on Ce2O3 Surfaces. *Topics in Catalysis*, **2019**, 62, 956-967	2.3	3
100	Oxygen Vacancies in Oxide Nanoclusters: When Silica Is More Reducible Than Titania. *Frontiers in Chemistry*, **2019**, 7, 37	5	0
99	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	1.9	1
98	X-Ray Diffraction and Theoretical Calculation-Supported Formation of Polymorphic Cocrystals Discovered Through Thermal Methods: A Case Study. *Journal of Pharmaceutical Sciences*, **2019**, 108, 3340-3347	3.9	12
97	Nanoparticle Assembling through Click Chemistry Directed by Mixed SAMs for Magnetic Applications. *ACS Applied Nano Materials*, **2019**, 2, 554-565	5.6	2
96	Theoretical analysis of the adsorption of ammonia-borane and their dehydrogenation products on the (001) surface of TiC and ZrC. *Surface Science*, **2019**, 680, 95-106	1.8	5
95	Can Supported Reduced Vanadium Oxides form H from CHOH? A Computational Gas-Phase Mechanistic Study. *Journal of Physical Chemistry A*, **2018**, 122, 1104-1113	2.8	5
94	Stability of mixed-oxide titanosilicates: dependency on size and composition from nanocluster to bulk. *Nanoscale*, **2018**, 10, 832-842	7.7	12

93	Periodic density functional theory study of maghemite (001) surface. Structure and electronic properties. *Surface Science*, **2018**, 677, 239-253	1.8	4
92	Properties of hydrated TiO and SiO nanoclusters: dependence on size, temperature and water vapour pressure. *Nanoscale*, **2018**, 10, 21518-21532	7.7	5
91	Breaking H with CeO: Effect of Surface Termination. *ACS Omega*, **2018**, 3, 16063-16073	3.9	28
90	Global optimisation of hydroxylated silica clusters: A cascade Monte Carlo Basin Hopping approach. *Computational and Theoretical Chemistry*, **2017**, 1102, 38-43	2	10
89	Application of dual descriptor to understand the activity of C u/Z r O catalysts in the water gas shift reaction. *Journal of Molecular Modeling*, **2017**, 23, 34	2	6
88	Periodic DFT Study of Rutile IrO2: Surface Reactivity and Catechol Adsorption. *Journal of Physical Chemistry C*, **2017**, 121, 13135-13143	3.8	24
87	Insights on hydride formation over cerium-gallium mixed oxides: A mechanistic study for efficient H2 dissociation. *Journal of Catalysis*, **2017**, 345, 258-269	7.3	23
86	Understanding iridium oxide nanoparticle surface sites by their interaction with catechol. *Physical Chemistry Chemical Physics*, **2017**, 19, 16151-16158	3.6	6
85	Scaling reducibility of metal oxides. *Theoretical Chemistry Accounts*, **2017**, 136, 1	1.9	45
84	Predicting size-dependent emergence of crystallinity in nanomaterials: titania nanoclusters versus nanocrystals. *Nanoscale*, **2017**, 9, 1049-1058	7.7	59
83	Butanethiol adsorption and dissociation on Ag (111): A periodic DFT study. *Surface Science*, **2016**, 646, 247-252	1.8	4
82	Nonlinear Fano interferences in open quantum systems: An exactly solvable model. *Physical Review A*, **2016**, 93,	2.6	7
81	Alkali Ion Incorporation into V2O5: a Noncovalent Interactions Analysis. *Journal of Physical Chemistry C*, **2016**, 120, 4259-4265	3.8	15
80	Photoactivity of Molecule-TiO2 Clusters with Time-Dependent Density-Functional Theory. *Journal of Physical Chemistry A*, **2016**, 120, 5115-24	2.8	22
79	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	3.8	41
78	Fano-Liouville spectral signatures in open quantum systems. *Physical Review Letters*, **2015**, 115, 113006	7.4	12
77	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	3.8	9
76	Platinum and platinum based nanoalloys synthesized by wet chemistry. *Faraday Discussions*, **2015**, 181, 19-36	3.6	8

75	Promoted ceria catalysts for alkyne semi-hydrogenation. *Journal of Catalysis*, **2015**, 324, 69-78	7.3	55
74	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	2	19
73	The role of dispersion forces in metal-supported self-assembled monolayers. *Computational and Theoretical Chemistry*, **2015**, 1053, 322-327	2	9
72	Understanding the Role of Oxygen Vacancies in the Water Gas Shift Reaction on Ceria-Supported Platinum Catalysts. *ACS Catalysis*, **2014**, 4, 2088-2096	13.1	130
71	Novel Delta-Ta2O5 Structure Obtained from DFT Calculations. *Journal of Physical Chemistry C*, **2014** , 118, 13652-13658	3.8	9
70	SERS as a Probe of Charge-Transfer Pathways in Hybrid Dye/Molecule/Metal Oxide Complexes. *Journal of Physical Chemistry C*, **2014**, 118, 3774-3782	3.8	24
69	Dopamine Adsorption on TiO2 Anatase Surfaces. *Journal of Physical Chemistry C*, **2014**, 118, 20688-20693	3.8	33
68	Probing Raman enhancement in a dopamine-Ti2O4 hybrid using stretched molecular geometries. *Journal of Physical Chemistry A*, **2014**, 118, 1196-202	2.8	8
67	Understanding How in Situ Generated Hydrogen Controls the Morphology of Platinum Nanoparticles. *Journal of Physical Chemistry C*, **2014**, 118, 9290-9298	3.8	10
66	Surface Reduction Mechanism of Cerium/Gallium Mixed Oxides with Enhanced Redox Properties. *Journal of Physical Chemistry C*, **2013**, 117, 8822-8831	3.8	24
65	Toward an understanding of the hydrogenation reaction of MO2 gas-phase clusters (M = Ti, Zr, and Hf). *Journal of Physical Chemistry A*, **2013**, 117, 5354-64	2.8	10
64	Hydration Dynamics for Vanadia/Titania Catalysts at High Loading: A Combined Theoretical and Experimental Study. *Journal of Physical Chemistry C*, **2013**, 117, 25535-25544	3.8	15
63	Unravelling the enhanced reactivity of bulk CeO2 doped with gallium: A periodic DFT study. *Chemical Physics Letters*, **2012**, 519-520, 69-72	2.5	12
62	Ionic interactions: Comparative topological approach. *Computational and Theoretical Chemistry*, **2012**, 998, 193-201	2	31
61	Theoretical and Experimental Study of Light Hydrocarbon Ammoxidation and Oxidative Dehydrogenation on (110)-VSbO4 Surfaces. *Journal of Physical Chemistry C*, **2012**, 116, 9132-9141	3.8	20
60	Revealing the Surface Reactivity of Zirconia by Periodic DFT Calculations. *Journal of Physical Chemistry C*, **2012**, 116, 6636-6644	3.8	50
59	Exploring Metal Oxides: A Theoretical Approach **2011**, 375-426		
58	Theoretical Investigation of the Hydrogenation of (TiO2)N Clusters (N = 1−10). *Journal of Physical Chemistry C*, **2011**, 115, 15890-15899	3.8	60

57	Hydrogen Adsorption and Diffusion on the Anatase TiO2(101) Surface: A First-Principles Investigation. *Journal of Physical Chemistry C*, **2011**, 115, 6809-6814	3.8	118
56	Combined ATR-FTIR and DFT Study of Cyclohexanone Adsorption on Hydrated TiO2 Anatase Surfaces. *Journal of Physical Chemistry C*, **2011**, 115, 14164-14172	3.8	20
55	Dynamics of Hydration in Vanadia□Titania Catalysts at Low Loading: A Theoretical and Experimental Study. *Journal of Physical Chemistry C*, **2011**, 115, 24133-24142	3.8	24
54	Theoretical study of H2 dissociation on a ZrO2 cluster. *Chemical Physics Letters*, **2011**, 503, 12-17	2.5	8
53	Comment on "Imaging of the hydrogen subsurface site in rutile TiO2". *Physical Review Letters*, **2010** , 104, 119603; author reply 119604	7.4	17
52	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	3.8	19
51	Hydrogen Adsorption on Monoclinic (1 11) and (1 01) ZrO2 Surfaces: A Periodic ab Initio Study. *Journal of Physical Chemistry C*, **2010**, 114, 11918-11923	3.8	25
50	Density functional theory study of the oxidation of methanol to formaldehyde on a hydrated vanadia cluster. *Journal of Computational Chemistry*, **2010**, 31, 2493-501	3.5	11
49	Ethylene glycol interaction on alkaline earth oxides: A periodic DFT study. *Catalysis Today*, **2010**, 152, 88-92	5.3	12
48	Correlation between theoretical and experimental investigations of the ammonia adsorption process on the (1 1 0)-VSbO4 surface. *Catalysis Today*, **2010**, 158, 178-185	5.3	20
47	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, 10864-70	4.8	53
46	Theoretical investigation of the inversion parameter in Co3□AlsO4 (s=0□) spinel structures. *Solid State Ionics*, **2009**, 180, 1011-1016	3.3	17
45	What do vanadium framework sites look like in redox model silicate zeolites?. *Microporous and Mesoporous Materials*, **2009**, 119, 137-143	5.3	41
44	Is There a Nanosize for the Activity of TiO2 Compounds?. *Journal of Physical Chemistry C*, **2009**, 113, 12186-12194	3.8	35
43	Characterization of Supported Vanadium Oxide Species on Silica: A Periodic DFT Investigation. *Journal of Physical Chemistry C*, **2009**, 113, 10740-10746	3.8	69
42	Stability of binary SAMs formed by omega-acid and alcohol functionalized thiol mixtures. *Langmuir*, **2009**, 25, 9980-5	4	30
41	Stability of formate species on beta-Ga2O3. *Physical Chemistry Chemical Physics*, **2009**, 11, 1397-405	3.6	51
40	Cation distributions on CoAl2O4 and Co2AlO4 spinels: pressure and temperature effects. *High Pressure Research*, **2008**, 28, 521-524	1.6	11

39	Stability of Hydroxylated (1 11) and (1 01) Surfaces of Monoclinic Zirconia: A Combined Study by DFT and Infrared Spectroscopy. *Journal of Physical Chemistry C*, **2008**, 112, 6469-6476	3.8	56
38	Reactivity of (TiO2)N Clusters (N = 1□10): Probing Gas-Phase Acidity and Basicity Properties. *Journal of Physical Chemistry C*, **2008**, 112, 16087-16095	3.8	60
37	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	3.8	44
36	Diffusion versus desorption: complex behavior of H atoms on an oxide surface. *ChemPhysChem*, **2008**, 9, 253-6	3.2	118
35	Reactivity of gas-phase, crystal and supported V2O5 systems studied using density functional theory based reactivity indices. *Chemical Physics Letters*, **2008**, 456, 59-63	2.5	44
34	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	5.3	35
33	A DFT study of methanol dissociation on isolated vanadate groups. *Catalysis Today*, **2008**, 139, 214-220	5.3	16
32	Effect of Alkali Doping on a V2O5/TiO2 Catalyst from Periodic DFT Calculations. *Journal of Physical Chemistry C*, **2007**, 111, 6411-6417	3.8	46
31	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	5.3	28
30	Periodic DFT study of the structural and electronic properties of bulk CoAl2O4 spinel. *Journal of Physical Chemistry B*, **2006**, 110, 988-95	3.4	60
29	Spin localization for NO adsorption on surface O atoms of metal oxides. *Catalysis Today*, **2006**, 113, 201-207	5.3	13
28	Reactivity of the V2O5□TiO2-anatase catalyst: role of the oxygen sites. *Topics in Catalysis*, **2006**, 41, 17-26	2.3	31
27	Migration of the subsurface C impurity in Pd(111). *Physical Review B*, **2005**, 71,	3.3	38
26	Lithium insertion and mobility in the TiO2-anatase/titanate structure: A periodic DFT study. *Journal of Electroanalytical Chemistry*, **2005**, 581, 216-223	4.1	47
25	Comparison of the reduction of metal oxide surfaces: TiO2-anatase, TiO2-rutile and SnO2-rutile. *Surface Science*, **2005**, 583, 107-117	1.8	91
24	Proton ordered cubic and hexagonal periodic models of ordinary ice. *Chemical Physics Letters*, **2005**, 409, 110-117	2.5	49
23	A DFT study on the hydrated V2O5-TiO2-anatase catalyst: stability of monomeric species. *Theoretical Chemistry Accounts*, **2005**, 114, 29-37	1.9	24
22	Restoring the band gap of metal oxide surfaces by redox adsorption. *Computational and Theoretical Chemistry*, **2004**, 709, 87-96		4

21	CO oxidation over anatase TiO2-(001). *Computational and Theoretical Chemistry*, **2004**, 709, 73-78		47
20	Modeling catalytic reduction of NO by ammonia over V2O5. *Surface Science Reports*, **2004**, 55, 169-236	12.9	71
19	Effect of relaxation on structure and reactivity of anatase (1 0 0) and (0 0 1) surfaces. *Surface Science*, **2004**, 552, 169-179	1.8	69
18	Electron-count control on adsorption upon reducible and irreducible clean metal-oxide surfaces. *Catalysis Today*, **2004**, 89, 269-278	5.3	49
17	Reactivity of the Oxygen Sites in the V2O5/TiO2Anatase Catalyst. *Journal of Physical Chemistry B*, **2004**, 108, 15679-15685	3.4	37
16	Theoretical Investigation of NO Oxidation over TiO2-Anatase. *Surface Review and Letters*, **2003**, 10, 175-182	1.2	22
15	Theoretical Study on the Molecular Mechanism for the Reaction of VO2+ with C2H4. *Journal of Physical Chemistry A*, **2003**, 107, 3107-3120	2.8	68
14	Ionization of HCl and HF in ice: a periodic DFT study. *Chemical Physics Letters*, **2003**, 369, 287-292	2.5	31
13	A periodic model for the V2O5□TiO2 (anatase) catalyst. Stability of dimeric species. *Surface Science*, **2003**, 526, 297-308	1.8	50
12	Adsorption on perfect and reduced surfaces of metal oxides. *Catalysis Today*, **2003**, 85, 125-143	5.3	127
11	An atom-in-molecules and electron-localization-function study of the interaction between O2 and VxOy+/VxOy (x = 1, 2, y = 1□5) clusters. *Theoretical Chemistry Accounts*, **2002**, 108, 12-20	1.9	19
10	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	1.8	92
9	The hierarchy of localization basins: a tool for the understanding of chemical bonding exemplified by the analysis of the VOx and VOx+ (x=1□4) systems. *Theoretical Chemistry Accounts*, **2001**, 105, 299-308	1.9	63
8	A theoretical study on the structure, energetics and bonding of VOx+ and VOx (x=1□4) systems. *Chemical Physics Letters*, **2001**, 333, 493-503	2.5	66
7	Theoretical study of ZnO (1010) and Cu/ZnO (1010) surfaces. *Chemical Physics Letters*, **2001**, 338, 224-230	2.5	34
6	Quantum-mechanical analysis of the equation of state of anatase TiO2. *Physical Review B*, **2001**, 64,	3.3	63
5	Static simulation of bulk and selected surfaces of anatase TiO2. *Surface Science*, **2001**, 490, 116-124	1.8	106
4	A Systematic Density Functional Theory Study of VxOy+ and VxOY (X = 2□4, Y = 2□10) Systems. *Journal of Physical Chemistry A*, **2001**, 105, 9760-9775	2.8	102

3	A theoretical analysis of adsorption and dissociation of CH3OH on the stoichiometric SnO2(110) surface. *Surface Science*, **1999**, 430, 213-222	1.8	65
2	The Subsurface Diffusion of Hydrogen on Rutile TiO2 Surfaces: A Periodic DFT Study. *Topics in Catalysis*,1	2.3	1
1	Elucidation of the IR of Cu and Mn substituted intraframework SiBEA zeolites. *Topics in Catalysis*,1	2.3	