Beatriz Irigoyen

List of Publications by Year
in descending order

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40	783	471061	552369
papers	citations	17	26
		h-index	g-index

42	42	42	905
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	Mn-Doped CeO₂: DFT+U Study of a Catalyst for Oxidation Reactions. Journal of Physical Chemistry C, 2013, 117, 18063-18073.	1.5	68
2	Theoretical and experimental study of methane steam reforming reactions over nickel catalyst. Applied Surface Science, 2007, 253, 4427-4437.	3.1	58
3	Preparation and characterization of Ce/Zr mixed oxides and their use as catalysts for the direct oxidation of dry CH4. Catalysis Today, 2005, 107-108, 53-59.	2.2	48
4	Reaction Pathway for Coke-Free Methane Steam Reforming on a Ni/CeO₂ Catalyst: Active Sites and the Role of Metalâ€“Support Interactions. ACS Catalysis, 2021, 11, 8327-8337.	5.5	39
5	Ce-Pr mixed oxides as active supports for Water-gas Shift reaction: Experimental and density functional theory characterization. Applied Catalysis A: General, 2014, 485, 123-132.	2.2	37
6	Nature of the Active Sites on Ni/CeO₂ Catalysts for Methane Conversions. ACS Catalysis, 2021, 11, 10604-10613.	5.5	37
7	DFT study of H2 adsorption on Pd-decorated single walled carbon nanotubes with C-vacancies. International Journal of Hydrogen Energy, 2012, 37, 10156-10164.	3.8	34
8	Experimental and theoretical study about sulfur deactivation of Ni/ CeO2 and Rh/CeO2 catalysts. Materials Chemistry and Physics, 2016, 172, 69-76.	2.0	32
9	A First-Principles Modeling of Ni Interactions on CeO₂â^'ZrO₂Mixed Oxide Solid Solutions. Journal of Physical Chemistry C, 2011, 115, 7456-7465.	1.5	28
10	The location of a hydrogen atom and hydrogen molecules in BCC Fe: an ASED-MO approach. Modelling and Simulation in Materials Science and Engineering, 1995, 3, 319-329.	0.8	24
11	Bonding in PdH2 and Pd2H2 systems adsorbed on carbon nanotubes: Implications for hydrogen storage. International Journal of Hydrogen Energy, 2014, 39, 8780-8790.	3.8	23
12	Oxidation of toluene to benzaldehyde over VSb0.8Ti0.2O4Effect of the operating conditions. Catalysis Today, 2001, 64, 179-187.	2.2	22
13	Redox behavior of a low-doped Pr-CeO2(111) surface. A DFT+U study. Applied Surface Science, 2017, 401, 206-217.	3.1	22
14	Unraveling the Origin of Ceria Activity in Waterâ€“Gas Shift by First-Principles Microkinetic Modeling. Journal of Physical Chemistry C, 2020, 124, 7823-7834.	1.5	21
15	Vanadium antimonate as a partial oxidation catalyst. Applied Catalysis A: General, 2003, 250, 279-285.	2.2	19
16	Methane oxidation reactions on MoO3(100): A theoretical study. Journal of Molecular Catalysis A, 1998, 129, 297-310.	4.8	18
17	The location of atomic hydrogen in an edge-dislocated BCC Fe. Journal Physics D: Applied Physics, 1998, 31, 2179-2183.	1.3	18
18	Segregation of H, C and B to Î£ = 5 (0 1 3) Î±-Fe grain boundary: A theoretical study. Applied Surface Science, 2006, 253, 1939-1945.	3.1	17

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19	Hydrogen on the Fe (1Ì„12) surface and hydrogen pairs near bcc mixed (a/2)[11Ì„1] dislocation: electronic structure. Surface Science, 2000, 466, 97-110.	0.8	16
20	The adsorption of toluene on Vâ€“Sb oxides. Theoretical aspects. Surface Science, 2003, 523, 252-266.	0.8	16
21	Density functional theory study of water interactions on Mn-doped CeO2(111) surface. Applied Surface Science, 2014, 313, 784-793.	3.1	16
22	Oxygen vacancy formation on the Ni/Ce0.75Zr0.25O2(111) surface. A DFT+U study. International Journal of Hydrogen Energy, 2012, 37, 14937-14944.	3.8	15
23	A DFT study of phenol adsorption on a low doping Mnâ€“Ce composite oxide model. Applied Surface Science, 2015, 359, 14-20.	3.1	15
24	The interaction of hydrogen with an Fe vacancy: a molecular orbital simulation. Journal Physics D: Applied Physics, 1996, 29, 1306-1309.	1.3	14
25	Electronic structure and bonding of hydrogen in a screw dislocated bcc Fe. Applied Surface Science, 2001, 172, 8-17.	3.1	14
26	A molecular orbital study of H interaction with an edge dislocation in Fe bcc. Modelling and Simulation in Materials Science and Engineering, 1997, 5, 357-363.	0.8	13
27	Adsorption Reactions of Toluene on the (110) Vanadium Antimonate Oxide Surface. Journal of Catalysis, 2001, 201, 169-182.	3.1	13
28	DFT insights into structural effects of Niâ€“Cu/CeO₂ catalysts for CO selective reaction towards waterâ€“gas shift. Physical Chemistry Chemical Physics, 2021, 23, 3826-3836.	1.3	12
29	Adsorption of ammonia on vanadiumâ€“antimony mixed oxides. Applied Surface Science, 2012, 258, 3617-3623.	3.1	10
30	Effect of Fe doped over Vâ€“Sb oxide catalyst in toluene selective oxidation. Catalysis Today, 2008, 133-135, 775-779.	2.2	9
31	Promoted methane activation on doped ceria via occupation of Pr(4f) states. Applied Surface Science, 2018, 458, 397-404.	3.1	9
32	CH3 and CH2 Oxidation Reactions on MoO3(100): Analysis of the Electronic Structure. Journal of Catalysis, 2000, 190, 14-21.	3.1	8
33	The influence of Mg on the C adsorption on Ni(100): A DFT study. Journal of Molecular Catalysis A, 2010, 315, 171-177.	4.8	7
34	Tuning the selectivity of cerium oxide for ethanol dehydration to ethylene. Applied Surface Science, 2022, 599, 153963.	3.1	7
35	The electronic structure of vanadium antimonate. Catalysis Today, 2005, 107-108, 40-45.	2.2	6
36	Catalytic behaviour of V-Sb-Ti mixed oxides in the vapour-phase reaction of ethylbenzene with air. Catalysis Today, 2005, 107-108, 444-450.	2.2	5

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37	Theoretical study of the influence of cation vacancies on the catalytic properties of vanadium antimonate. Applied Surface Science, 2008, 254, 5837-5843.	3.1	4
38	The Effect of Metalâ€“Cation Vacancies on Vanadium Antimonate Surface Properties. A Theoretical Study. Journal of Physical Chemistry C, 2013, 117, 20548-20556.	1.5	4
39	Partial oxidation of toluene to benzaldehyde over vanadium antimonate catalysts doped with titanium. The influence of the antimony content over the deactivation process.. Studies in Surface Science and Catalysis, 2001, , 383-389.	1.5	3
40	Propylene Adsorption On a Nonstoichiometric VSbO₄(110) Surface. Journal of Physical Chemistry C, 2015, 119, 4967-4975.	1.5	2