Beatriz Irigoyen

List of Publications by Citations

39 papers	607 citations	15 h-index	22 g-index
42 ext. papers	680 ext. citations	5.4 avg, IF	3.96 L-index

#	Paper	IF	Citations
39	Mn-Doped CeO2: DFT+U Study of a Catalyst for Oxidation Reactions. *Journal of Physical Chemistry C* , **2013**, 117, 18063-18073	3.8	53
38	Theoretical and experimental study of methane steam reforming reactions over nickel catalyst. *Applied Surface Science*, **2007**, 253, 4427-4437	6.7	47
37	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	5.3	38
36	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	5.1	33
35	DFT study of H2 adsorption on Pd-decorated single walled carbon nanotubes with C-vacancies. *International Journal of Hydrogen Energy*, **2012**, 37, 10156-10164	6.7	30
34	A First-Principles Modeling of Ni Interactions on CeO2ZrO2 Mixed Oxide Solid Solutions. *Journal of Physical Chemistry C*, **2011**, 115, 7456-7465	3.8	26
33	Experimental and theoretical study about sulfur deactivation of Ni/ CeO2 and Rh/CeO2 catalysts. *Materials Chemistry and Physics*, **2016**, 172, 69-76	4.4	23
32	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	2	23
31	Bonding in PdH2 and Pd2H2 systems adsorbed on carbon nanotubes: Implications for hydrogen storage. *International Journal of Hydrogen Energy*, **2014**, 39, 8780-8790	6.7	21
30	Oxidation of toluene to benzaldehyde over VSb0.8Ti0.2O4: Effect of the operating conditions. *Catalysis Today*, **2001**, 64, 179-187	5.3	21
29	Vanadium antimonate as a partial oxidation catalyst. *Applied Catalysis A: General*, **2003**, 250, 279-285	5.1	17
28	Methane oxidation reactions on MoO3(100): A theoretical study. *Journal of Molecular Catalysis A*, **1998**, 129, 297-310		16
27	The adsorption of toluene on VSb oxides. Theoretical aspects. *Surface Science*, **2003**, 523, 252-266	1.8	16
26	The location of atomic hydrogen in an edge-dislocated BCC Fe. *Journal Physics D: Applied Physics*, **1998**, 31, 2179-2183	3	16
25	Redox behavior of a low-doped Pr-CeO2(111) surface. A DFT+U study. *Applied Surface Science*, **2017** , 401, 206-217	6.7	15
24	Segregation of H, C and B to Σ5 (0 1 3) αFe grain boundary: A theoretical study. *Applied Surface Science*, **2006**, 253, 1939-1945	6.7	15
23	Hydrogen on the Fe (1 12) surface and hydrogen pairs near bcc mixed (a/2)[11 1] dislocation: electronic structure. *Surface Science*, **2000**, 466, 97-110	1.8	15

22	Electronic structure and bonding of hydrogen in a screw dislocated bcc Fe. *Applied Surface Science*, **2001**, 172, 8-17	6.7	14
21	A DFT study of phenol adsorption on a low doping MnCe composite oxide model. *Applied Surface Science*, **2015**, 359, 14-20	6.7	13
20	Density functional theory study of water interactions on Mn-doped CeO2(1 1 1) surface. *Applied Surface Science*, **2014**, 313, 784-793	6.7	13
19	Adsorption Reactions of Toluene on the (110) Vanadium Antimonate Oxide Surface. *Journal of Catalysis*, **2001**, 201, 169-182	7.3	13
18	Oxygen vacancy formation on the Ni/Ce0.75Zr0.25O2(111) surface. A DFT+U study. *International Journal of Hydrogen Energy*, **2012**, 37, 14937-14944	6.7	12
17	The interaction of hydrogen with an Fe vacancy: a molecular orbital simulation. *Journal Physics D: Applied Physics*, **1996**, 29, 1306-1309	3	12
16	Reaction Pathway for Coke-Free Methane Steam Reforming on a Ni/CeO Catalyst: Active Sites and the Role of Metal-Support Interactions. *ACS Catalysis*, **2021**, 11, 8327-8337	13.1	12
15	Unraveling the Origin of Ceria Activity in Water Gas Shift by First-Principles Microkinetic Modeling. *Journal of Physical Chemistry C*, **2020**, 124, 7823-7834	3.8	11
14	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	2	11
13	Adsorption of ammonia on vanadium antimony mixed oxides. *Applied Surface Science*, **2012**, 258, 3617-3623	6.7	9
12	Nature of the Active Sites on Ni/CeO Catalysts for Methane Conversions. *ACS Catalysis*, **2021**, 11, 10604-10613	13.1	9
11	Promoted methane activation on doped ceria via occupation of Pr(4f) states. *Applied Surface Science*, **2018**, 458, 397-404	6.7	7
10	The influence of Mg on the C adsorption on Ni(1 0 0): A DFT study. *Journal of Molecular Catalysis A*, **2010**, 315, 171-177		7
9	Effect of Fe doped over V Sb oxide catalyst in toluene selective oxidation. *Catalysis Today*, **2008**, 133-135, 775-779	5.3	7
8	CH3 and CH2 Oxidation Reactions on MoO3(100): Analysis of the Electronic Structure. *Journal of Catalysis*, **2000**, 190, 14-21	7.3	6
7	The electronic structure of vanadium antimonate. *Catalysis Today*, **2005**, 107-108, 40-45	5.3	5
6	Theoretical study of the influence of cation vacancies on the catalytic properties of vanadium antimonate. *Applied Surface Science*, **2008**, 254, 5837-5843	6.7	4
5	Catalytic behaviour of V-Sb-Ti mixed oxides in the vapour-phase reaction of ethylbenzene with air. *Catalysis Today*, **2005**, 107-108, 444-450	5.3	4

4	DFT insights into structural effects of Ni-Cu/CeO catalysts for CO selective reaction towards water-gas shift. *Physical Chemistry Chemical Physics*, **2021**, 23, 3826-3836	3.6	4
3	The Effect of Metal Cation Vacancies on Vanadium Antimonate Surface Properties. A Theoretical Study. *Journal of Physical Chemistry C*, **2013**, 117, 20548-20556	3.8	3
2	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	1.8	3
1	Propylene Adsorption On a Nonstoichiometric VSbO4(110) Surface. *Journal of Physical Chemistry C*, **2015**, 119, 4967-4975	3.8	2